A METHOD FOR DESIGNING A COMPOUND BASED ON THE THREE DIMENSIONAL STRUCTURE OF PHOSPHOINOSITIDE DEPENDENT PROTEIN KINASE 1 (PDK1)

METHODS

5 Cross-reference to Related Application

The present application is the US national phase under 35 USC 371 of International Application No. PCT/GB03/02509, filed June 9, 2003, and published in the English language as WO 03/104481.

10 Reference to Sequence Listing

The present application incorporates by reference the sequence listing submitted as an ASCII text filed via EFS-Web on January 18, 2010. The Sequence Listing is provided as a file entitled 8400121_1.txt, created on January 18, 2010, which is 4 Kb in size.

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Field of the Invention

The present invention relates to protein kinase catalytic domain structures and mutants and screening assays making use thereof.

20 Background of the Invention

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) is a key protein kinase, regulating activity of a group of related protein kinases through phosphorylation. These kinases include isoforms of Protein Kinase B (also known as Akt) [Brazil and Hemmings, 2001, Scheid and Woodgett, 2001], p70 ribosomal S6 kinase (S6K) [Alessi et al., 1997, Volarevic and Thomas, 2001], p90 ribosomal S6 Kinase (RSK) [Frodin and Gammeltoft, 1999] and the serum and glucocorticoid induced-protein kinase (SGK) [Lang and Cohen, 2001]. These enzymes are stimulated by hormones and growth factors and phosphorylate regulatory proteins mediating the various physiological effects of these agonists.

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PDK1 possesses an N-terminal kinase catalytic domain and a C-terminal pleckstrin homology (PH) domain [Alessi et al., 1997,Stephens et al., 1998]. PDK1 activates its substrates by phosphorylating these kinases at their activation loop (reviewed in [Alessi, 2001,Toker and Newton, 2000]). The phosphorylation of PKB by PDK1 is dependent upon prior activation of the phosphoinositide 3-kinase (PI-3-kinase) and the production of the second messenger, phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃) which binds to the PH domains of PDK1 and PKB. This does not activate either PKB or PDK1 but instead recruits and co-localises these enzymes at the plasma membrane.

Unlike PKB, the other PDK1 substrates described thus far do not interact with PtdIns(3,4,5)P₃ nor is the rate at which they are phosphorylated by PDK1 further enhanced by the binding of PDK1 to PtdIns(3,4,5)P₃. Instead the ability of PDK1 to phosphorylate S6K, SGK and RSK is promoted by phosphorylation of these enzymes at a residue located C-terminal to the kinase catalytic domain in a region known as the hydrophobic motif [Alessi et al., 1997,Kobayashi and Cohen, 1999, Pullen et al., 1998]. The kinases that phosphorylate the hydrophobic motif of S6K and SGK are unknown but as the phosphorylation of this residue *in vivo* is dependent on PI-3-kinase activation, the hydrophobic motif kinases and/or the hydrophobic motif phosphatases may be regulated by PtdIns(3,4,5)P₃. In the case of RSK isoforms, phosphorylation by the ERK1/ERK2 MAP kinases induce phosphorylation of the hydrophobic motif (reviewed in Frodin and Gammeltoft, 1999).

PDK1 belongs to the same subfamily of protein kinases as its substrates, termed the AGC protein kinases as they are related to the cAMP dependent protein kinase (PKA)/cGMP dependent protein kinase/Protein kinase C

(PKC). PKA is the only AGC kinase whose crystal structure has been solved. Like all protein kinases, its catalytic core possesses an N-terminal lobe consisting mainly of β -sheet and a predominantly α -helical Cterminal lobe [Taylor et al., 1992, Husen and Kuriyan, 2002]. The ATP binding site is located in between the 2 lobes [Johnson et al., 2001, Knighton et al., 1991]. At the very C-terminus, PKA possesses an extended loop that terminates in the sequence FXXF (SEQ ID NO:1) which resembles the first part of the hydrophobic motif phosphorylation site of S6K and SGK (FXXFS/TY, SEQ ID NO:2) in which the Ser/Thr is the phosphorylated residue [Biondi et al., 2000]. In the structure of PKA, the FXXF motif (SEO ID NO:1) is buried in a hydrophobic pocket in the small lobe of the PKA catalytic domain [Knighton et al., 1991] and mutation of either of the Phe residues drastically reduces PKA activity towards a peptide substrate [Etchebehere et al., 1997]. Unlike other AGC kinases, PDK1 does not possess a hydrophobic motif C-terminal to its catalytic domain. However, there is evidence that PDK1 possesses a hydrophobic pocket in the small lobe of its catalytic domain similar to that in PKA. We have biochemically demonstrated that the interaction of PDK1 with four of its substrates (S6K1, SGK1, PK ζ and PKC related kinase-2 (PRK2)) is reduced or abolished by mutation of residues predicted to form part of this pocket [Balendran et al., 2000, Biondi et al., 2000]. Furthermore, mutation of a central residue in the predicted pocket, Leu 155, prevented PDK1 from phosphorylating and activating S6K1 and SGK1 without affecting its ability to phosphorylate either PKB or a short peptide substrate that encompasses the activation loop of PKB (T308tide) [Biondi et al., 2000]. The hydrophobic pocket on the kinase domain of PDK1 has been termed the "PIF-pocket" after the name of the first AGC-kinase hydrophobic motif-containing peptide (PDK1 Interacting Fragment) that was found to bind PDK1 [Balendran et al., 1999a]. It has been suggested that the PIF-pocket in PDK1 functions as a docking site, enabling PDK1 to interact with some of its.physiological

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substrates. Furthermore, there is evidence that phosphorylation of the hydrophobic motif of S6K1, SGK and RSK2 [Balendran et al., 1999b,Biondi et al., 2001, Frodin et al., 2000] promotes the interaction of these enzymes with PDK1. These findings suggest that the PIF-pocket on PDK1 could contain a phosphate binding site promoting the binding of PDK1 to a subset of substrates (S6K, SGK and RSK) once these enzymes have been phosphorylated at their hydrophobic motif. This would result in a physiological phosphate dependent interaction. In addition there is evidence that occupancy of the PIF-pocket activates PDK1 as peptides that encompass the hydrophobic motif of PRK2 [Biondi et al., 2000] and RSK [Frodin et al., 2000] induce a 4-6-fold activation of PDK1.

Previous predicted structures PDK1 catalytic domain were obtained using homology modelling methods based upon structural information available from the catalytic domain of PKA (Biondi et al., 2000). These predictions of the PDK1 catalytic domain structure were thus biased towards the catalytic domain from which the structural information was obtained.

Summary of the Invention

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We have determined a crystal structure for the kinase domain of the AGC family protein kinase PDK. The structure defines the PIF-pocket and reveals an adjacent possible phosphate binding site. Furthermore, we have performed structure-based mutagenesis and biochemical analysis which support the existence of such a phosphate-binding site. This may mediate the phosphate dependent docking interaction with substrates such as (for PDK1) S6K and SGK. We have used a novel algorithm to define the conformational state of the crystallised PDK1 relative to all the reported structures of PKA, which shows that while PDK1 has all the signs of being in an active form in the crystal, its overall conformation is in-between and 'open' and 'closed' state. We have also determined crystal structures for

the kinase domain of PDK1 in complex with modulators of PDK1 activity. On the basis of this work we provide drug screening methods and mutated protein kinase molecules (which are useful in, for example, drug screening methods).

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A first aspect of the invention provides a method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

20 Brief Description of the Drawings

Figure 1 provides an overview of the PDK1 structure.

Figures 2A and 2B show the PIF-pocket.

Figure 3 shows a structure-based sequence alignment

Figures 4A-C show PDK1 binding & activation studies.

25 Figures 5A and 5B show interactions of regulatory phosphates with the α C helix.

Figures 6A and 6B show essential dynamics.

Figure 7 shows alignment of AGC protein kinase family members.

Figure 8 shows staurosporine and UCN-01 electron density. Figure 9 shows details of the inhibitor binding sites.

Detailed Description of the Invention

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The term PDK1 as used herein includes a polypeptide (a PDK1 polypeptide) comprising the amino acid sequence identified as PDK1 in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776-789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714, or a variant, fragment, fusion or derivative thereof, or a fusion of a said variant or fragment or derivative, for example as described in WO98/41638, incorporated herein by reference. It is preferred that the said PDK1 polypeptide is a protein kinase. It is preferred that the said PDK1 polypeptide is a protein kinase that is capable of phosphorylating a threonine residue that lies in a Thr-Phe-Cys-Gly-Thr-Xaa-Glu-Leu consensus motif (where the underlined Thr corresponds to the threonine that is phosphorylated by PDK1 and Xaa is a variable residue, SEQ ID NO:9), and preferably that is capable of phosphorylating PKB, for example PKBα, at residue Thr308. The rate at which the said PDK1 polypeptide is capable of phosphorylating a threonine residue as described above may be increased in the presence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂ but it will be appreciated that this is not essential. The said polypeptide may be capable of phosphorylating the equivalent residues to Thr308 of PKBα on PKC isoforms (LeGood et al (1998) Science 281: 2042-2045; et al (1998) Curr. Biol. 8: 1069-1077; Dutil et al (1998) Curr. Biol. 8:1366-1375), p70 S6 kinase (Alessi et al (1998) Curr. Biol. 8: 69-81; Pullen et al (1998) Science **279**, 707-710), SGK (sequence given in Webster et al. (1993) Mol. Cell. Biol. 13, 1031-2040; equivalent residues identified in US application no 112217 filed on 14 December 1998; GB 9919676.8, filed on 19 August 1999, and Kobayashi & Cohen (1999)) and PKA (Cheng et al. (1998) Proc. Natl. Acad. Sci. USA 95: 9849-9854). It may further be

preferred that the substrate specificity and/or other characteristics of the said PDK1 polypeptide *in vitro* may be substantially as reported in Alessi D.R *et al* (1997) *Curr. Biol.* 7: 261-269, Alessi D.R *et al* (1997) *Curr. Biol.* 7: 776-789, Stokoe D *et al* (1997) *Science* 277: 567-570 or Stephens L *et al* (1998) *Science* 279: 710-714.

We have found that a fragment of PDK1 consisting essentially of residues equivalent to residues 51 to 359 of full length human PDK1 is particularly beneficial for determining a structure for the catalytic domain of PDK1. This fragment has, for example, protein kinase activity and surprisingly beneficial solubility and stability characteristics which make it particularly suitable for structural studies, for example formation of crystals which may be analysed by X-ray crystallography methods. Other fragments of PDK1 were surprisingly found to be unsuitable for crystallisation, as discussed in Example 5.

It is particularly preferred that the structure is one determined for the fragment consisting of residues 51 to 359 of full length human PDK1. The fragment may comprise an N-terminal or C-terminal fusion polypeptide (ie amino acid sequence not derived from PDK1), though this is preferably of less than or equal to about 10, 5, 4, 3, 2 or 1 amino acids. For example, it is particularly preferred that the structure is one determined for a polypeptide consisting residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro (or less preferably other sequence forming part of a protease cleavage site) preceding the methionine corresponding to Met51 of human PDK1. A further preferred structure is one determined for the fragment consisting essentially of residues 71 to 359 of full length human PDK1 (or residues equivalent thereto), which also has protein kinase activity.

It is particularly preferred that the structure is one determinable by a method as described in Example 1, for example a structure obtainable by X-ray analysis from a crystal obtainable using a mother liquor solution comprising ammonium sulphate, preferably between 1.8 and 2.2M. It is particularly preferred that the mother liquor solution is of pH 7 to 9, preferably 7 to 8.5, most preferably pH8.5, and comprises ammonium sulphate and preferably ATP. Crystals may form in the absence of ATP but better crystals may be obtained in the presence of ATP. Preferably the crystal is obtainable using a mother liquor solution containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP. Further preferred details of the crystallisation and X-ray analysis are described in Example 1, for example as partially summarised in Table 1 (shown in Example 1).

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It is particularly preferred that the structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure based or modelled on such a structure or co-ordinates. The co-ordinates shown in Example 2 are for the PDK1 fragment (SEQ ID NO:102) with all alternate side chains. The co-ordinates shown in Example 3 are for the PDK1 fragment (SEQ ID NO:102) without alternate side chains. The co-ordinates shown in Example 4 are for the dimer of the PDK1 fragment (SEQ ID NO:102), without alternate side chains; chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

The structure may be one determined following crystallisation in the presence of a known or potential interactor with PDK1 or modulator of PDK1 activity (as discussed further below), for example a known or potential inhibitor of PDK1 activity. For example, the structure may be one determined following crystallisation in the presence of a known protein kinase inhibitor, for example an inhibitor that binds at the ATP binding site,

for example an ATP-competitive inhibitor, for example staurosporine or a staurosporine derivative, for example UCN-01. Examples of such crystallisation techniques and analysis are given in Example 6, and examples of co-ordinates are given in Examples 7 and 8. Example 7 represents the co-ordinates of PDK1 fragment (SEQ ID NO:102) co-crystallised with Staurosporine, whereas in Example 8, the co-ordinates of PDK1 fragment (SEQ ID NO:102) co-crystallised with UCN-01.

It will be appreciated that some variation in crystallisation conditions (for example different mother liquors) may be required for co-crystallisation with different molecules. Techniques for investigating suitable crystallisation conditions in each case will be well known to those skilled in the art.

A further aspect of the invention provides a crystalline form of a polypeptide as defined in any of the preceding aspects of the invention, for example a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 or a fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro preceding the methionine corresponding to Met51 of human PDK1; a polypeptide consisting of residues 71 to 359 of full length human PDK1 or a fusion thereof.

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The crystalline form may further comprise co-crystallised molecule, for example a known or potential interactor with PDK1 or modulator of PDK1 activity, or a test compound whose properties *vis a vis* PDK1 may not be known. For example, the co-crystallised molecule, for example test compound, may be a molecule that is known to modulate protein kinase

activity, or may already be known to modulate PDK1 protein kinase activity. For example, the co-crystallised molecule may be staurosporine, the staurosporine derivative UCN-01 (7-hydroxyl staurosporine) or other staurosporine derivative.

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Such co-crystallisation and structures determined from co-crystallised molecules may be useful in molecular modelling and in determining features of the polypeptide and compound that are important for interaction. This may be useful in designing or selecting further test compounds, for example as discussed in Example 6.

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In one embodiment it is preferred that the modelled molecule is predicted to bind to a region of the structure termed the "PIF binding pocket", the "phosphate binding pocket" and/or the α C helix (residues equivalent to 123-136 of full length human PDK1), particularly the residue equivalent to Arg 131 of full length human PDK1, or interacting regions. As discussed in Example 1, the PIF binding pocket is considered to be formed by residues including Lys115, Ile118, Ile119 on the α B helix, Val124, Val127 on the α C helix and Leu 155 on β -sheet 5. The phosphate binding pocket is considered to be formed by residues including Lys76, Arg 131, Thr 148 and Gln150. Residues of the α C helix that are considered to interact either with phosphate bound in the phosphate binding site or intermolecularly with phosphorylated Ser241 of PDK1 include Arg131 (phosphate binding site) and Arg 129 and His126 (phosphorylated Ser241). Glu 130 is involved in binding the α -phosphate of the bound ATP, and Val124 and Val127 form part of the PIF binding pocket, as discussed in Example 1.

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It is preferred that the compound is for modulating the protein kinase activity of PDK1. The protein kinase activity of PDK1 that is modulated

may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu ("PDK1" activity, SEQ ID NO:9). Alternatively or in addition, the modulated activity may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Phe-Xaa-Xaa-Phe-Ser/Thr-Phe/Tyr ("PDK2" activity. SEQ ID NO:11). The substrate polypeptide may be, for example, a PKB, SGK, p70 S6 kinase, PKC or (in relation only to phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu (SEQ ID NO:9) PKA polypeptide. The modulated protein kinase activity may be towards PKB or other PHdomain-comprising/phosphoinositide-binding substrate of PDK1; or SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY (SEQ ID NO:2); or an artificial substrate such as T308tide (which comprises the sequence of PKB which is phosphorylated by PDK1) or PDKtide (which comprises the sequence of PKB which is phosphorylated by PDK1 (eg T308tide) fused to a sequence mimicking a phosphorylated hydrophobic motif ie FXXFZY (SEQ ID NO: 2), in which Z is a negatively charged (for example acidic) residue (eg PIFtide)). Such substrates for PDK1 are discussed, for example, in WO Other activities of PDK1 that may be modulated include 01/44497. interactions with other polypeptides or phosphoinositides and/or intramolecular interactions.

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It is preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of the PDK1 is a three-dimensional structure of at least a part of the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, and a compound that is predicted to interact with the said PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of

PDK1 is selected. Alternatively, the compound may bind to a portion of said PDK1 polypeptide that is not the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, for example so as to interfere with the binding of the ATP or substrate polypeptide or their access to the catalytic site. In a still further example, the compound may bind to a portion of PDK1 so as to decrease said polypeptide's activity by an allosteric effect. This allosteric effect may be an allosteric effect that is involved in the natural regulation of PDK1's activity.

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It is further preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure of the part of the protein kinase catalytic domain of PDK1 that is defined by residues Lys115, Ile118, Ile119 (on the αB helix), Val124, Val127 (on the αC helix) and Leu 155 (on β -sheet 50 and/or residues Lys76, Arg 131, Thr 148 and Gln150 and/or residues Arg131, Arg 129, His126, Glu 130 of full-length human PDK1 and a compound that is predicted to interact with the said part of the protein kinase catalytic domain is selected.

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For example, it is preferred if the portions of the structure of PDK1 shown in Figures 1 and 2 as forming the PIF binding pocket and/or phosphate binding pocket and/or α C helix interactions (for example with phosphoserine241) are compared with the structure of the candidate compound.

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A further aspect of the invention provides a method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, is selected.

The three-dimensional structure of a compound may be compared with the three-dimensional structure of the hydrophobic and/or phosphate binding pocket and/or αC helix or region interacting therewith, as appropriate. A compound that can interact with the hydrophobic pocket and/or phosphate binding pocket, in particular residues noted above as defining such regions, in a similar manner (for example similar separation and/or type of interaction ie hydrophobic or ionic, and/or similar cumulative energy of interaction) to an interacting polypeptide such as S6K-pHM may be selected. Methods of assessing the interaction are well known to those skilled in the art and are discussed further below.

The three-dimensional structures that are compared may be, as appropriate, predicted or modelled three-dimensional structures (for example on the basis of a PDK1 structure as referred to above, for example as represented

by the co-ordinates given in Examples 2, 3 or 4 or 6 or 7) or may be three-dimensional structures that have been determined, for example by techniques such as X-ray crystallography, as well known to those skilled in the art. The three-dimensional structures may be displayed by a computer in a two-dimensional form, for example on a computer screen. The comparison may be performed using such two-dimensional displays.

The following relate to molecular modelling techniques: Blundell *et al* (1996) Stucture-based drug design *Nature* **384**, 23-26; Bohm (1996) Computational tools for structure-based ligand design *Prog Biophys Mol Biol* **66(3)**, 197-210; Cohen *et al* (1990) *J Med Chem* **33**, 883-894; Navia *et al* (1992) *Curr Opin Struct Biol* **2**, 202-210.

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The following computer programs, for example, may be useful in carrying out the method of this aspect of the invention: GRID (Goodford (1985) J Med Chem 28, 849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al (1991) Proteins: Structure, Function and Genetics 11, 29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al (1990) Proteins: Structure, Function and Genetics 8, 195-202; available from Scripps Research Institute, La Jolla, CA); DOCK (Kuntz et al (1982) J Mol Biol 161, 269-288; available from the University of California, San Francisco, CA); LUDI (Bohm (1992) J Comp Aid Molec Design 6, 61-78; available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al (1991) Tetrahedron 47, 8985; available from Molecular Simulations, Burlington, MA); LeapFrog (available from Tripos Associates, St Louis, MO); Gaussian 92, for example revision C (MJ Frisch, Gaussian, Inc., Pittsburgh, PA ©1992); AMBER, version 4.0 (PA Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994); and Insight II/Discover (Biosym Technologies Inc., San

Diego, CA ©1994). Programs may be run on, for example, a Silicon GraphicsTM workstation, Indigo²TM or IBM RISC/6000TM workstation model 550.

Several *in silico* methods could be employed, for example, via a substructure search for new ligands using programmes such as CHEM DRAW or CHEM FINDER. The basic structure of the natural ligand (for example a phosphorylated hydrophobic motif peptide such as S6K-pHM) capable of binding to PDK1 (or other protein kinase) is taken (or predicted) and various structural features of it (for example the hydrophobic and negatively charged entities) are submitted to a programme which will searches a set of chemical company catalogues for chemicals containing this substructure.

These compounds are then screened by eye for groups that could not interact with the PIF/phosphate binding pockets (or the αC residues/interacting region) because, for example, they are too large or have steric or charge hindrance, and those are discarded. The remaining chemicals are submitted to a PRODRG server and topologies/co-ordinates for these chemicals are created. These chemicals are modelled into the structure, from which chemicals that are possibly able to bind to the PIF/phosphate binding site domain/ α C helix/interacting region are selected. Further details of the PRODRG programme are available at http://davape1.bioch.dundee.ac.uk/programs/prodrg/prodrg.html in the art, for example, from Daan van Aalten Laboratory.

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These compounds may then be ordered or synthesised and assessed, for one or more of ability to bind to and/or modulate PDK1 (or other protein kinase) activity. The compounds may be crystallised with the PDK1 or other protein kinase protein and the structure of any complex determined, as illustrated in Examples 6 to 8.

An alternative approach is to use PRODRG: a tool for generating GROMOS/MOL2/WHATIF topologies and hydrogen atom positions from small molecule PDB files. We take the natural ligand and computationally vary all possible groups at each site on the ligand, with a variety of new groups while the protein co-ordinates and the ligand back-bone co-ordinates remain fixed the results can then be screened for hindrance and repulsion, and the molecules are obtained either through catalogues or made.

As noted above, the selected or designed compound may be synthesised (if not already synthesised) or purified and tested for its effect on the relevant hydrophobic/phosphate pocket-containing protein kinase, for example its effect on the protein kinase activity. The compound may be tested in a screening method of the invention or other screening method. The compound may be formulated for pharmaceutical use, for example for use in *in vivo* trials in animals or humans, or for use in agriculture, for example as an antifungal agent.

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It may be useful to analyse a protein kinase structure (for example a structure determined or predicted for a complex of the protein kinase with a binding partner) in order to determine the activation state of the structure. This may be useful in further modelling binding of the binding partner to the protein kinase in other activation states, and in predicting how the binding partner may affect the activation state of the protein kinase or compete with other potential binding partners. It may also be useful in designing and assessing derivatives of the binding partner.

Thus, a further aspect of the invention provides a method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates. The method may further comprise the step of classifying the activation state

of the structure as "open", "closed" or "intermediate". Details of the analysis, which involves the generation of eigenvectors and associated eigenvalues are given in Example 1. The analysis makes use of techniques described in Amadei *et al* (1993) Essential dynamics of proteins. *Proteins* 17, 412-425.

The hydrophobic/phosphate pocket-containing protein kinase may be PDK1. Alternatively, it may be an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2. Hydrophobic/phosphate pocket-containing protein kinases and their EMBL database accession numbers are listed in Table I. Sequences considered to form the phosphate binding pocket from representative hydrophobic/phosphate pocket-containing protein kinases are shown in Figure 5. All AGC family protein kinases other than PKA may be hydrophobic/phosphate pocket-containing protein kinases, as defined above. In addition to the protein kinases shown in Figure 7, rhodopsin and G-protein coupled receptor protein kinases, for example, may possibly also have a hydrophobic/phosphate pocket as defined above.

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The terms SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, for example, as used herein include a polypeptide (a SGK, PKB, PKA, p70S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 polypeptide) comprising the amino acid sequence identified as a SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, respectively, in the relevant EMBL database records indicated in Table 2.

Table 2

Activation or T- AGC Hydrophobic Accession

	Loop	Motif	number
consensus:	$\underline{T}FCGTxxYxAPD$	FxxF <u>S</u> Y	
	(SEQ ID NO:41)	(SEQ ID NO:42)	
	L E	$Y\underline{T}F$	
ΡΚΒα	TFCGTPEYLAPE	FPQF <u>S</u> Y	(Y15056)
	(SEQ ID NO:45)	(SEQ ID NO:46)	
РКВβ	TFCGTPEYLAPE	FPQF <u>S</u> Y	(P31751)
	(SEQ ID NO:47)	(SEQ ID NO:48)	
ΡΚΒγ	TFCGTPEYLAPE	FPQF <u>S</u> Y	(AF135794)
	(SEQ ID NO:49)	(SEQ ID NO:50)	
SGK1	TFCGTPEYLAPE	FLGF <u>S</u> Y	(AAD41091)
	(SEQ ID NO:51)	(SEQ ID NO:52)	
SGK2	TFCGTPEYLAPE	FLGF <u>S</u> Y	(AF169034)
	(SEQ ID NO:53)	(SEQ ID NO:54)	
SGK3	TFCGTPEYLAPE	FLGF <u>S</u> Y	(AF169035)
	(SEQ ID NO:55)	(SEQ ID NO:56)	
ΡΚCα	TFCGTPDYIAPE	FEGF <u>S</u> Y	(4506067)
	(SEQ ID NO:57)	(SEQ ID NO:58)	
ΡΚСβΙ	TFCGTPDYIAPE	FAGF <u>S</u> Y	(4506069)
	(SEQ ID NO:59)	(SEQ ID NO:60)	
PKCβII	TFCGTPDYIAPE	FEGF <u>S</u> F	(P05127)
	(SEQ ID NO:61)	(SEQ ID NO:62)	
ΡΚСγ	TFCGTPDYIAPE	FGGF <u>T</u> Y	(P05129)
	(SEQ ID NO:63)	(SEQ ID NO:64)	
ΡΚCδ	TFCGTPDYIAPE	FAGF <u>S</u> F	(5453970)
	(SEQ ID NO:65)	(SEQ ID NO:66)	
ΡCΚζ	TFCGTPNYIAPE	FEGFEY	(4506079)
	(SEQ ID NO:67)	(SEQ ID NO:68)	
PKCι	TFCGTPNYIAPE	FEGFEY	(4506071)
	(SEQ ID NO:69)	(SEQ ID NO:68)	

PRK1	TFCGTPEFLAPE	FLDFDF	(AAC50209)
	(SEQ ID NO:71)	(SEQ ID NO:72)	
PRK2	$\underline{T}FCGTPEFLAPE$	FRDFDY	(AAC50208)
	(SEQ ID NO:73)	(SEQ ID NO:74)	
p70-S6Kα	$\underline{T}FCGTIEYMAPE$	FLGF <u>T</u> Y	(AAA36410)
	(SEQ ID NO:75)	(SEQ ID NO:76)	
p70-S6Kβ	$\underline{T}FCGTIEYMAPE$	FLGF <u>T</u> Y	(4506739)
	(SEQ ID NO:77)	(SEQ ID NO:78)	
p90-RSK1	\underline{S} FCGTVEYMAPE	FRGF <u>S</u> F	(I38556)
	(SEQ ID NO:79)	(SEQ ID NO:80)	
p90-RSK2	\underline{S} FCGTVEYMAPE	FRDF <u>S</u> F	(P51812)
	(SEQ ID NO:81)	(SEQ ID NO:82)	
p90-RSK3	<u>S</u> FCGTIEYMAPE	FRGF <u>S</u> F	(CAA59427)
	(SEQ ID NO:83)	(SEQ ID NO:84)	
MSK1	<u>S</u> FCGTIEYMAPD	FQGY <u>S</u> F	(AAC31171)
	(SEQ ID NO:85)	(SEQ ID NO:86)	
MSK2	\underline{S} FCGTIEYMAPE	FQGY <u>S</u> F	(AAC67395)
	(SEQ ID NO:87)	(SEQ ID NO:88)	
PDK1	<u>s</u> fvgtaqyvspe	(1)	(AF017995)
	(SEQ ID NO:89)		

Table 2. Alignment of the amino acid sequences surrounding the T-loop and the hydrophobic motif of AGC kinases. All the sequences and accession numbers are from human proteins. The underlined residues correspond to those that become phosphorylated. Footnotes: (1) PDK1 does not possess a hydrophobic motif.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the

protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor *et al* (1999) *Curr Biol* **9**, 186-197.

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The PDK1 may also be a polypeptide with the amino acid sequence of residues 51 to 359 or 404 (or 71 to 360) of full-length human PDK1; this may comprise the protein kinase domain of PDK1, as described in Example 2. The PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may also be Myc epitope-tagged or His-tagged, as described in Example 1. The p70 S6 kinase, for example, may have a His tag at its N-terminus and/or may lack the carboxy terminal 104 residues (p70 S6K-T2). The PDK1 or SGK may be a *Saccharomyces cerevisiae* homologue, for example Pkh1 or Pkh2 (PDK1 homologues) or Ypk1 or Yrk2 (SGK homologues), as described in Casamayor *et al* (1999) *Curr Biol* **9**, 186-197.

It is particularly preferred, although not essential, that the variant or fragment or derivative or fusion of the PDK1, or the fusion of the variant or fragment or derivative has at least 30% of the enzyme activity of full-length human PDK1 with respect to the phosphorylation of full-length human PKBα on residue Thr308 or SGK1 on residue Thr 256 in either the presence or absence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂. It is more preferred if the variant or fragment or derivative or fusion of the said protein kinase, or the fusion of the variant or fragment or derivative has at least 50%, preferably

at least 70% and more preferably at least 90% of the enzyme activity of

PDK1 with respect to the phosphorylation of PKBα or SGK1. However, it will be appreciated that variants or fusions or derivatives or fragments which are devoid of enzymatic activity may nevertheless be useful, for example by interacting with another polypeptide. Thus, variants or fusions or derivatives or fragments which are devoid of enzymatic activity may be useful in a binding assay, which may be used, for example, in a method of the invention in which modulation of an interaction of a mutated PDK1 of the invention and optionally also PDK1 with a interacting polypeptide or compound, for example an interacting polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr (SEQ ID NO:92), for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr (SEQ ID NO:93), for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Asp/Glu-Phe/Tyr (SEQ ID NO:94) or Phe/Tyr-Xaa-Xaa-Phe/Tyr-PhosphoSer/PhosphoThr-Phe/Tyr (SEQ ID NO:94) is measured.

It is preferred that the variant or fragment or derivative or fusion of the said hydrophobic/phosphate binding pocket-containing protein kinase, or the fusion of the variant or fragment or derivative comprises a hydrophobic pocket and a phosphate binding pocket in the position equivalent to the hydrophobic and phosphate binding pocket of human PDK1, as discussed further below.

Equivalent preferences apply to a variant or fragment or derivative or fusion of the SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 (for example), or the fusion of the variant or fragment or derivative, with the substitution in relation to SGK, PKB and p70S6 kinase of the peptide substrate Crosstide (GRPRTSSFAEG, SEQ ID NO:96), or for PKB and SGK of the peptide substrate RPRAATF; the substitution in relation to PKA of the peptide substrate Kemptide (LRRASLG, SEQ ID NO:97); the substitution in relation to PKC isoforms and PRK1/2 of histone H1; and the

substitution in relation to MSK1/2 or p90-RSK1/2/3 of CREBtide (EILSRRPSYRK, SEQ ID NO:98).

By "variants" of a polypeptide we include insertions, deletions and substitutions, either conservative or non-conservative. In particular we include variants of the polypeptide where such changes do not substantially alter the activity of the said polypeptide, for example the protein kinase activity of PDK1, as described above.

By "conservative substitutions" is intended combinations such as Gly, Ala; Val, Ile, Leu; Asp, Glu; Asn, Gln; Ser, Thr; Lys, Arg; and Phe, Tyr.

The three-letter amino acid code of the IUPAC-IUB Biochemical Nomenclature Commission is used herein, with the exception of the symbol Zaa (negatively charged amino acid). In particular, Xaa represents any amino acid. It is preferred that Xaa and Zaa represent a naturally occurring amino acid. It is preferred that at least the amino acids corresponding to the consensus sequences defined above are L-amino acids.

It is particularly preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of PDK1 referred to above (or the sequence for SGK (including SGK1, 2 and 3), PKB, PKA or p70 S6 kinase, for example, as appropriate, referred to above), more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 80%, in further preference at least 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above.

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It is still further preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase, as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of the catalytic domain, particularly the residues forming the hydrophobic pocket, of PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) in the appropriate sequence referred to above, more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 83 or 85%, in still further preference at least 80% in further preference at least 83 or 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above. It will be appreciated that the catalytic domain of a protein kinase-related polypeptide may be readily identified by a person skilled in the art, for example using sequence comparisons as described below.

The percent sequence identity between two polypeptides may be determined using suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group and it will be appreciated that percent identity is calculated in relation to polypeptides whose sequence has been aligned optimally.

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The alignment may alternatively be carried out using the Clustal W program (Thompson *et al* (1994) *Nucl Acid Res* **22**, 4673-4680). The parameters used may be as follows:

Fast pairwise alignment parameters: K-tuple(word) size; 1, window size; 5, gap penalty; 3, number of top diagonals; 5. Scoring method: x percent.

Multiple alignment parameters: gap open penalty; 10, gap extension penalty; 0.05.

Scoring matrix: BLOSUM.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor *et al* (1999) *Curr Biol* 9, 186-197.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide that is capable of interacting with a polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr_(SEQ ID NO:92), preferably Phe-Xaa-Xaa-Phe/Tyr, more preferably Phe-Xaa-Xaa-Phe, still more preferably Phe/Tyr-Xaa-Xaa-Phe/Tyr-ZXaa-Phe/Tyr (SEQ ID NO:93) or Phe/Tyr-Xaa-Xaa-Phe/Tyr-COOH, for example the polypeptide PIF or PIFtide, as defined below. Further preferences for the said polypeptide are as given above.

The protein kinase activity of PKB, SGK or p70 S6 kinase that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Arg-Xaa-Arg-Xaa-Xaa-Ser/Thr (SEQ ID NO:100). The polypeptide may be Glycogen Synthase Kinase 3 (GSK3), 40 S ribosomal subunit S6, BAD, 6-phosphofructo-2-kinase, phosphodiesterase3b, human caspase 9, endothelial nitric oxide synthase or BRCA1.

A compound identified by a method of the invention may modulate the ability of the protein kinase to phosphorylate different substrates, for example different naturally occurring polypeptides, to different extents. The compound may inhibit the protein kinase activity in relation to one substrate but may increase the protein kinase activity in relation to a second substrate. For example, the protein kinase activity of PDK1 may be modulated to a different extent for PKB when compared with SGK, p70 S6 kinase and/or PKC.

It will be appreciated that the modulatory, for example inhibitory action of a compound found to bind (or inhibit binding of a polypeptide or compound) to the protein kinase may be confirmed by performing an assay of enzymic activity (for example PDK1 and/or PDK2 protein kinase activity) in the presence of the compound.

By "hydrophobic pocket-containing protein kinase having a hydrophobic pocket (PIF binding pocket) in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150," is meant a polypeptide having an amino acid sequence identifiable as that of a protein kinase catalytic domain, and further having a predicted or determined three-dimensional structure that includes a hydrophobic pocket corresponding to the region indicated in Example 1 as the PIF binding pocket, and a pocket corresponding to the region indicated in Example 1 as the phosphate binding pocket. The hydrophobic pocket and phosphate binding pockets in PDK1 do not overlap with the ATP or phosphorylation site binding sites on PDK1.

It is preferred that the protein kinase has identical or conserved residues that are equivalent to Lys 115, Ile118, Ile119, Val124, Val127 and/or Leu 155 of human PDK1, more preferably at least Lys115 and Leu155 of human PDK1, most preferably an identical residue equivalent to Leu155. Thus, for example, the protein kinase may have a Lys residue at the position equivalent to Lys115 of PDK1 and/or a Leu residue at the position equivalent to Leu155 of PDK1. It is preferred that the protein kinase does not have an Ala at the position equivalent to Lys115 and/or a Ser, Asp or Glu at the position equivalent to Leu155 of PDK1.

It is further preferred that the protein kinase has identical or conserved residues that are equivalent to Lys76, Arg131, Thr148 and/or Gln 150 of human PDK1, more preferably at least Lys76 and Gln150 of human PDK1, most preferably an identical residue equivalent to Gln150. Figure 5B shows an alignment of examples of protein kinases considered to have a phosphate binding pocket at the position equivalent to the said phosphate binding pocket of PDK1. Sequence conservation/preferred residues at the positions identified are discussed further in Example 1.

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An amino acid sequence may be identifiable as that of a protein kinase catalytic domain by reference to sequence identity or similarities of three dimensional structure with known protein kinase domains, as known to those skilled in the art.

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Protein kinases show a conserved catalytic core, as reviewed in Johnson *et al* (1996) *Cell*, **85**, 149-158 and Taylor & Radzio-Andzelm (1994) *Structure* **2**, 345-355. This core folds into a small N-terminal lobe largely comprising anti-parallel β -sheet, and a large C-terminal lobe which is mostly α -helical.

A deep cleft at the interface between these lobes is the site of ATP binding, with the phosphate groups near the opening of the cleft.

Protein kinases also show conserved sequences within this catalytic core, and the residue equivalent to a given residue of, for example, PDK1, may be identified by alignment of the sequence of the kinase with that of known kinases in such a way as to maximise the match between the sequences. The alignment may be carried out by visual inspection and/or by the use of suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group, which will also allow the percent identity of the polypeptides to be calculated. The Align program (Pearson (1994) in: Methods in Molecular Biology, Computer Analysis of Sequence Data, Part II (Griffin, AM and Griffin, HG eds) pp 365-389, Humana Press, Clifton).

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The comparison of amino acid sequences or three dimension structure (for example from crystallography or computer modelling based on a known structure) may be carried out using methods well known to the skilled man, for example as described in WO 01/44497.

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MAP kinase, MEK1, Cdk2 and Erk2 (for example) are not protein kinases having a hydrophobic pocket in the position equivalent to the hydrophobic (PIF binding) pocket of PDK1. MEK1, Cdk2 and ERK2 may have a larger hydrophobic pocket which interacts with an amino acid sequence motif (which may be Phe-Xaa-Phe-Pro, SEQ ID NO:101) which is not Phe-Xaa-Xaa-Phe (SEQ ID NO:99). Thus, these protein kinases do not have a hydrophobic pocket in the position equivalent to the said hydrophobic (PIF-binding) pocket of PDK1.

A further aspect of the invention provides a mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated. It is preferred that the said protein kinase is PDK1. The said protein kinase may alternatively be, for example, SGK, PKB or p70 S6 kinase. It is particularly preferred that the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala. The mutated protein kinase may be useful in determining whether a polypeptide or compound interacts with the hydrophobic (PIF binding) pocket or phosphate binding pocket of the unmutated protein kinase. For example, the abilities of a compound (including polypeptide) to bind to the mutated and unmutated protein kinase, or to modulate the activity of the protein kinase towards one or more substrates of the protein kinase, may be measured and compared.

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The mutated protein kinase may alternatively or in addition be mutated at a residue forming part of the "hydroxyl-pocket" discussed in Example 6, for example the residue equivalent to Thr222 and/or Gln 220 of full length human PDK1. These residues are involved in the binding of the UCN-01 7-hydroxyl group.

A further aspect of the invention provides a polynucleotide encoding a mutated protein kinase of the invention. A still further aspect of the invention provides a recombinant polynucleotide suitable for expressing a

mutated protein kinase of the invention. A yet further aspect of the invention provides a host cell comprising a polynucleotide of the invention.

A further aspect of the invention provides a method of making a mutated protein kinase of the invention, the method comprising culturing a host cell of the invention which expresses said mutated protein kinase and isolating said mutated protein kinase.

A further aspect of the invention provides a mutated protein kinase obtainable by the above method.

Examples of these aspects of the invention are provided in Example 1, and may be prepared using routine methods by those skilled in the art, for example as described in WO 00/35946.

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For example, the above mutated protein kinase may be made by methods well known in the art and as described below and in Example 1 or 2, for example using molecular biology methods or automated chemical peptide synthesis methods.

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It will be appreciated that peptidomimetic compounds may also be useful. Thus, by "polypeptide" or "peptide" we include not only molecules in which amino acid residues are joined by peptide (-CO-NH-) linkages but also molecules in which the peptide bond is reversed. Such retro-inverso peptidomimetics may be made using methods known in the art, for example such as those described in Mézière *et al* (1997) *J. Immunol.* 159, 3230-3237, incorporated herein by reference. This approach involves making pseudopeptides containing changes involving the backbone, and not the orientation of side chains. Retro-inverse peptides, which contain NH-CO

bonds instead of CO-NH peptide bonds, are much more resistant to proteolysis.

Similarly, the peptide bond may be dispensed with altogether provided that an appropriate linker moiety which retains the spacing between the $C\alpha$ atoms of the amino acid residues is used; it is particularly preferred if the linker moiety has substantially the same charge distribution and substantially the same planarity as a peptide bond.

It will be appreciated that the peptide may conveniently be blocked at its Nor C-terminus so as to help reduce susceptibility to exoproteolytic digestion.

The invention further provides a method of identifying a compound that modulates the protein kinase activity of a protein kinase having a hydrophobic pocket and phosphate binding pocket in the positions equivalent to the hydrophobic (PIF binding) pocket and phosphate binding pocket of PDK1, as defined above (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to the said mutated protein kinase of the invention.

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The method may further comprise determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated at the said residue. When the protein kinase is PDK1, it may lack a functional PH domain (ie it may lack a PH domain capable of binding a phosphoinositide).

It will be appreciated that the protein kinase or mutated protein kinase may be a fusion protein comprising a tag, for example to aid purification, for example a GST tag, as described in Example 1. The capability of the said PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) polypeptide with regard to interacting with or binding to a polypeptide or other compound may be measured by any method of detecting/measuring a protein/protein interaction or other compound/protein interaction, as discussed further below. Suitable methods include methods analagous to those described in Example 1, as well as other methods, for example yeast two-hybrid interactions, co-purification, ELISA, co-immunoprecipitation and surface plasmon resonance methods. Thus, the said PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may be considered capable of binding to or interacting with a polypeptide or other compound if an interaction may be detected between the said PDK1 polypeptide and the said interacting polypeptide by ELISA, co-immunoprecipitation or surface plasmon resonance methods or by a yeast two-hybrid interaction or copurification method, for example as described in Example 1.

It is preferred that the interaction can be detected using a surface plasmon resonance method, as described in Example 1. The interacting polypeptide (for example a polypeptide comprising a phosphorylated "hydrophobic motif", for example S6K-pHM; see example 1) may be immobilised on the test surface, for example it can be coupled through amino groups to a SensorChip CM5TM, according to the manufacturer's instructions, or a biotinylated polypeptide can be bound to an avidin coated SensorChip SA. The protein kinase (at concentrations between, for example 0 and between 10μM and 1.0μM, for example 2μM) is then injected over the surface and steady state binding determined in each case. From these measurements a K_d can be determined. It is preferred that the interaction has a K_d of less than 8μM, more preferably less than 5μM, 2μM, 1μM, 500nM, 300nM, 200nM or 100nM, for example about 150nM. Alternatively, a K_d can be determined for a polypeptide or other compound in competition with the immobilised polypeptide (or other compound). The protein kinase (for

example at a concentration of 0.5µM) is mixed with free polypeptide (for example, at concentrations between 0 and 3µM) and the mixture injected over the immobilised polypeptides. The steady state binding is determined in each case, from which the K_d of the interaction can be determined using the Cheng-Prescott relationship. Alternatively, the interaction may be expressed in terms of an observed response or relative observed responses, measured in terms of mass of protein bound to the surface, as described in Example 2. For example, the polypeptide may be immobilised by amino coupling to a SensorChip CM5 and each protein kinase (for example different mutated protein kinases, as discussed below) for example at a concentration of 1.0µM or a range of concentrations, injected over the immobilised polypeptide. Alternatively, the polypeptide may be immobilised on a SA SensorChip and each protein kinase, for example at a concentration of 40nM or a range of concentrations injected over the immobilised polypeptide. The steady state response for each protein kinase is determined, for example expressed in Response Units (RU). 1000RU corresponds to 1 ng/mm² of protein bound to the surface. A response of less than 10RU may indicate that no interaction has taken place. A response of at least 10RU may indicate that the immobilised and injected molecules interact with each other.

It will be appreciated that the above methods may be used to determine whether a particular polypeptide or compound interacts with a protein kinase or mutated protein kinase.

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The effect of the compound on the rate or degree of phosphorylation of a hydrophobic pocket and/or phosphate binding pocket-dependent substrate may be determined. A compound may be selected that decreases the protein kinase activity of the said protein kinase, for example PDK1,

towards a hydrophobic pocket-dependent substrate or a phosphate binding pocket-dependent substrate and does not affect or increases the protein kinase activity towards a hydrophobic pocket or phosphate binding pocket-independent substrate, for example PKB when the kinase is PDK1. An activator of PDK1 may mimic insulin and may be useful in treating diabetes or obesity, and may protect cells from apoptosis.

Compounds that bind specifically to the phosphate binding site may activate PDK1 (or other AGK kinase having a phosphate binding site). Also compounds that bind to the residues forming part of the pohsphate binding site might transduce the negative effect and inhibit the kinase activity. A compound interacting with the phosphate binding site of PDK1 may be an activator, but only of a subset of substrates. Some substrates of PDK1 require the interaction with the phosphate binding site, such as S6K and SGK.

To generate a specific molecule that could bind to the phosphate and/or PIF-binding pocket of PDK1 a anti-idiotype strategy using combinatorial RNA libraries could be employed. Previous studies have established that Combinatorial RNA libraries can be used to isolate specific ligands, called aptamers, for virtually any target molecule by a procedure probably best known as SELEX (Ellington, A. D., and Szostak, J. W. (1990) Nature 346, 818-822; Tuerk, C., and Gold, L. (1990) Science 249, 505-510). Using this approach RNA molecules that interact with antibodies raised against PIFtide or peptides that encompass the hydrophobic motif of AGC kinases which are phosphorylated at their hydrophobic motif would be selected (preferably antibodies that are specific for the phosphorylated form ie bind the phosphorylated form but not the non-phosphorylated form). These RNA species then may have the intrinsic conformation to interact with the phosphate binding (and possibly also the PIF-binding) pocket(s) of PDK1.

Antibodies to the phosphate binding pocket may be produced. For example, animals could be immunised with wild type PDK1. Serum could then be purified with a column where the resin is coated with wild type PDK1 used for the immunisation. Specific antibodies could then be passed through columns coated with mutant PDK1 molecules differing only in that they have specific mutations in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala. Antibodies that don't bind to this mutant will either be specific antibodies that recognise the specific motifs or antibodies that are sensitive to the conformational changes associated with these mutations. The opposite development could also be performed: antibodies against a mutant PDK1 having a specific mutation(s) in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala, could be produced and the serum further purified through columns coated with wild type PDK1.

Thus, a further aspect of the invention provides an antibody reactive with the phosphate binding pocket of PDK1 or other hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150. A further aspect of the invention provides an antibody reactive with PDK1 or other phosphate-binding pocket—containing protein kinase as defined above but not with the said protein kinase mutated at the phosphate binding site, or *vice versa*. A further aspect of the invention provides a method for preparing or selecting an antibody wherein the antibody is prepared or selected against a said protein kinase (for example

PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.

By the term "antibody" is included synthetic antibodies and fragments and variants (for example as discussed above) of whole antibodies which retain the antigen binding site. The antibody may be a monoclonal antibody, but may also be a polyclonal antibody preparation, a part or parts thereof (for example an F_{ab} fragment or F(ab')₂) or a synthetic antibody or part thereof. Fab, Fv, ScFv and dAb antibody fragments can all be expressed in and secreted from *E. coli*, thus allowing the facile production of large amounts of the said fragments. By "ScFv molecules" is meant molecules wherein the V_H and V_L partner domains are linked via a flexible oligopeptide. IgG class antibodies are preferred.

Suitable monoclonal antibodies to selected antigens may be prepared by known techniques, for example those disclosed in "Monoclonal Antibodies: A manual of techniques", H. Zola (CRC Press, 1988) and in "Monoclonal Hybridoma Antibodies: techniques and Applications", JGR Hurrell (CRC Press, 1982), modified as indicated above. Bispecific antibodies may be prepared by cell fusion, by reassociation of monovalent fragments or by chemical cross-linking of whole antibodies. Methods for preparing bispecific antibodies are disclosed in Corvalen *et al*, (1987) *Cancer Immunol. Immunother.* **24**, 127-132 and 133-137 and 138-143.

A general review of the techniques involved in the synthesis of antibody fragments which retain their specific binding sites is to be found in Winter & Milstein (1991) *Nature* **349**, 293-299.

For example, an antibody that does not bind PDK1 Arg131Ala could be specifically recognising this residue in the phosphate binding site, but could

also be recognising specifically the inactive conformation of PDK1, which is stabilised by Arg 131. The opposite development could also be performed: antibodies against a mutant PDK1 Arg131Ala could be produced and the serum further purified through columns coated with wild type PDK1. In this way, antibodies may be prepared that would either not be able to interact with the phosphate binding site Arg 131 but only when a small residue is in its place, or antibodies that are probes for the active conformation of PDK1. These conformational probes could be used in high throughoutput screenings, HTS, in the search of compounds that are capable of modifying the conformation of the given protein kinase. Antibodies could have been produced with previous knowledge to detect active protein kinases by immunising with active protein kinases, but in those cases, the antibodies would have recognised also the phosphorylation events that make a protein kinase be active. In the methodology here described using antibodies, the conformational probes could be easily isolated. Furthermore, antibodies obtained from an active protein kinase (with overall modifications that make it active) could be further purified through a column coated with the inactive protein kinase (keeping the non bound fraction) and then further purifyied on a column coated with a protein kinase consisting of an activating mutation (such as R131A in the case of PDK1), retaining the specifically bound fraction, which could be an active conformation probe. This type of approach could also allow the development of conformation specific probes by the use of activating or inhibiting mutations.

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A further aspect of the invention provides a kit of parts useful in carrying out a method according to the preceding aspect of the invention, comprising (1) a mutated protein kinase of the invention and (2) the protein kinase which is not a mutated said protein kinase as defined above.

The protein structures described herein (for example with the co-ordinates shown in Examples 2, 3 or 4, or structures modelled thereon) may be useful in designing further reagents that may be useful in drug screening assays or characterisation of protein kinase activity or regulation. For example, such structures may be useful in designing mutants that may be useful in FRETbased activities, for example in which surface residues near to binding sites are mutated to cysteines to allow coupling of chromophores. For example, the cysteine residue may be fluorescently-labelled, and a change in fluorescence intensity or frequency may be detected in an assay. Any thiolreactive fluorophore, for example BADAN (see, for example, Wadum et al Fluorescently labeled bovine acyl-CoA binding protein – an acyl-CoA sensor. Interaction with CoA and acyl-CoA esters and its use in measuring free acyl CoA esters and non-esterified fatty acids (NEFA); Hammarstrom et al (2001) Biophys J **80(6)**, 2867-2885; Schindel et al (2001) Eur J Biochem 268(3), 800-808), could be used to label the cysteine. alternative suitable fluorophore is Acrylodan (Richieri et al (1992) J Biol *Chem* **267(33)**, 23495-23501).

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It will be appreciated that the invention provides screening assays for drugs which may be useful in modulating, for example either enhancing or inhibiting, the protein kinase activity of a protein kinase (for example, the protein kinase activity towards a particular substrate) having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of Protein Kinase A (PKA) that is defined by residues including Lys76, Leu116, 25 Val80 and/or Lys111 of full-length mouse PKA, for example PDK1, SGK, PKB, PKA or p70 S6 kinase, for example the PDK1 or PDK2 activity (as discussed above) of PDK1. The compounds identified in the methods may

themselves be useful as a drug or they may represent lead compounds for the design and synthesis of more efficacious compounds.

The compound may be a drug-like compound or lead compound for the development of a drug-like compound for each of the above methods of identifying a compound. It will be appreciated that the said methods may be useful as screening assays in the development of pharmaceutical compounds or drugs, as well known to those skilled in the art.

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The term "drug-like compound" is well known to those skilled in the art, and may include the meaning of a compound that has characteristics that may make it suitable for use in medicine, for example as the active ingredient in a medicament. Thus, for example, a drug-like compound may be a molecule that may be synthesised by the techniques of organic chemistry, less preferably by techniques of molecular biology or biochemistry, and is preferably a small molecule, which may be of less than 5000 daltons. A drug-like compound may additionally exhibit features of selective interaction with a particular protein or proteins and be bioavailable and/or able to penetrate cellular membranes, but it will be appreciated that these features are not essential.

The term "lead compound" is similarly well known to those skilled in the art, and may include the meaning that the compound, whilst not itself suitable for use as a drug (for example because it is only weakly potent against its intended target, non-selective in its action, unstable, difficult to synthesise or has poor bioavailability) may provide a starting-point for the design of other compounds that may have more desirable characteristics.

It is appreciated that screening assays which are capable of high throughput operation are particularly preferred. Examples may include cell based

assays and protein-protein binding assays. An SPA-based (Scintillation Proximity Assay; Amersham International) system may be used. For example, beads comprising scintillant and a substrate polypeptide or interacting polypeptide may be prepared. The beads may be mixed with a sample comprising ³²P- or ³³P-γ-labelled PDK1 or other protein kinase or mutated protein kinase (as defined above) and with the test compound. Conveniently this is done in a 96-well or 384-well format. The plate is then counted using a suitable scintillation counter, using known parameters for ³²P or ³³P SPA assays. Only ³²P or ³³P that is in proximity to the scintillant, i.e. only that bound to the substrate or interacting polypeptide that is bound to the beads, is detected. Variants of such an assay, for example in which the substrate or interacting polypeptide is immobilised on the scintillant beads *via* binding to an antibody or antibody fragment, may also be used.

It will be understood that it will be desirable to identify compounds that may modulate the activity of the protein kinase *in vivo*. Thus it will be understood that reagents and conditions used in the method may be chosen such that the interactions between, for example, the said protein kinase and the interacting polypeptide, are substantially the same as between the human protein kinase and a naturally occurring interacting polypeptide comprising the said amino acid sequence. It will be appreciated that the compound may bind to the protein kinase, or may bind to the interacting polypeptide.

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The compounds that are tested in the screening methods of the assay or in other assays in which the ability of a compound to modulate the protein kinase activity of a protein kinase, for example a hydrophobic pocket-containing protein kinase, as defined above, may be measured, may be compounds that have been selected and/or designed (including modified)

using molecular modelling techniques, for example using computer techniques.

A further aspect of the invention is a compound identified or identifiable by the above selection/design methods of the invention, for example an RNA molecule or antibody identifiable as defined above.

A still further aspect of the invention is a compound (or polypeptide or polynucleotide) of the invention or identified or identifiable by the above selection/design methods of the invention, for use in medicine. Conditions or diseases in which such compounds, polypeptides or polynucleotides may be useful are indicated below.

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The compound (or polypeptide or polynucleotide) may be administered in any suitable way, usually parenterally, for example intravenously, intraperitoneally or intravesically, in standard sterile, non-pyrogenic formulations of diluents and carriers. The compound (or polypeptide or polynucleotide) may also be administered topically, which may be of particular benefit for treatment of surface wounds. The compound (or polypeptide or polynucleotide) may also be administered in a localised manner, for example by injection. The compound may be useful as an antifungal (or other parasitic, pathogenic or potentially parasitic or pathogenic organism) agent.

A further aspect of the invention is the use of a compound (or polypeptide or polynucleotide) as defined above in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket, as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6

kinase/PRK2/PKC signalling. The patient may be in need of inhibition of a said hydrophobic/phosphate binding pocket-containing kinase in an infecting organism, for example the patient may have a fungal infection for which treatment is required. The compound may inhibit the infecting organism's (for example fungal) hydrophobic/phosphate binding pocket-containing protein kinase, but may not inhibit the patient's equivalent hydrophobic/phosphate binding pocket-containing protein kinase.

A further aspect of the invention is a method of treating a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound (or polypeptide or polynucleotide) as defined above.

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A compound that is capable of reducing the activity of PKC, for example PKCβ, PRK1 or 2, PDK1 (ie the PDK1 and/or the PDK2 activity), PKB, SGK or p70 S6 kinase may be useful in treating cancer. PDK1, for example *via* PKB and/or SGK, may be capable of providing a survival signal that protects cells from apoptosis induced in a variety of ways (reviewed in Cross *et al* (1995) *Nature* **378**, 785-789 and Alessi & Cohen (1998) *Curr. Opin. Genetics. Develop.* **8**, 55-62). Thus, such compounds may aid apoptosis. Reduction of the activity of PDK1, PKB, SGK and/or p70 S6 kinase may promote apoptosis and may therefore be useful in treating cancer. Conditions in which aiding apoptosis may be of benefit may also include resolution of inflammation.

A compound is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase may be useful in treating diabetes or obesity, or may be

useful in inhibiting apoptosis. Increased activity of PDK1, PKB, SGK or p70 S6 kinase may lead to increased levels of leptin, as discussed above, which may lead to weight loss; thus such compounds may lead to weight loss. For example, such compounds may suppress apoptosis, which may aid cell survival during or following cell damaging processes. It is believed that such compounds are useful in treating disease in which apoptosis is involved. Examples of such diseases include, but are not limited to, mechanical (including heat) tissue injury or ischaemic disease, for example stroke and myocardial infarction, neural injury and myocardial infarction. Thus the patient in need of modulation of the activity of PDK1, PKB, SGK or p70 S6 kinase may be a patient with cancer or with diabetes, or a patient in need of inhibition of apoptosis, for example a patient suffering from tissue injury or ischaemic injury, including stroke.

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Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identified or identifiable by the screening methods of the invention.

A still further invention provides a use of a compound identifiable by the screening methods of the invention in the manufacture of a medicament for treating an ischaemic disease in a patient.

Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identifiable by the screening methods of the invention.

If the patient is a patient in need of promotion of apoptosis, for example a patient with cancer, it is preferred that the compound of the invention that is

used in the preparation of the medicament is capable of reducing the activity of PDK1, PKB, SGK or p70 S6 kinase. If the patient is a patient with diabetes or a patient in need of inhibition of apoptosis, for example a patient with ischaemic disease, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase.

All documents referred to herein are hereby incorporated by reference.

The invention is now described in more detail by reference to the following, non-limiting, Figures and Examples.

Figure legends

15 1. Overview of the PDK1 structure.

The PDK1 kinase domain backbone is shown in a ribbon representation, with the secondary structure elements for residues 74-163 in the lower half of the Figure and for residues 164- 358 in the upper part of the Figure. Helix αG , encompassing residues 287-295 (which makes a crystal contact to a symmetry related PDK1 molecule, Fig. 2), is at the bottom right of the Figure. Key residues discussed in the text are shown as a sticks model. ATP is shown as a sticks model. A simulated annealing |Fo -|Fc`, ϕ calc map is shown in black, contoured at 3 σ . The phosphoserine and the sulphate discussed in the text are also shown.

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2. The PIF-pocket

A. A surface representation of the putative PIF binding pocket is shown and compared to the pocket interacting with the C-terminal FXXF (SEQ ID NO: 1) motif in PKA. For PDK1, the αG helix of a symmetry-related molecule

is shown as a ribbon, in PKA the C-terminus is also shown as a ribbon. Aromatic amino acids buried in the pocket are shown as sticks; further side chains interacting with the pocket are also shown as sticks. Helix α C is also shown as a ribbon in both PDK1 and PKA (at bottom of images). In PDK1, the ordered sulphate ion and basic residues interacting with it are also shown.

B. A stereo image of the residues lining the PIF-pocket is shown. The PDK1 backbone is shown as a grey ribbon. Side chains are shown as sticks. Hydrogen bonds to the sulphate ion are shown as black dotted lines.

3. Structure-based sequence alignment

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The sequences of PKA (SEQ ID NO: 103) and PDK1 (SEQ ID NO:102) are aligned according to a structural superposition performed in WHAT IF [Vriend, 1990]. Sequence numbering is according to PDK1. β-strands (arrows) and α-helices (bars) are shown for the PDK1 structure according to a DSSP [Kabsch and Sander, 1983] secondary structure assignment, and labelled consistent with the secondary structure element names proposed for PKA [Taylor and Radzioandzelm, 1994]. Residues lining the PIF-pocket are indicated with a black dot. Residues hydrogen bonding the sulphate ion are indicated by arrows. The PDK1 residues equivalent to Ser53 and Gly186 in PKA, are labelled with an asterisk.

4. PDK1 binding & activation studies

Binding and activation of wild type and mutant forms of PDK1 to a phosphopeptide derived from the hydrophobic motif of S6K1. The binding of the wild type (wt) PDK1 and indicated mutants to a phosphopeptide comprising the hydrophobic motif of S6K1 (S6K-pHM: SESANQVFLGFT*YVAPSV, where T* indicates phospho-threonine, SEQ

<u>ID NO:104</u>) was analysed by surface plasmon resonance as described in the Materials and Methods.

A. The sensor chip SA was coated with 12RUs of the biotinylated S6K-pHM peptide and the binding was analysed following injection of 270 nM wild type PDK1, PDK1 [T148A] and PDK1 [K76A]. No detectable binding to S6K-pHM was observed using PDK1 [R131A] or PDK1 [Q150] (data not shown).

B. As in **A.** except that binding was analysed over a range of PDK1 concentrations (2-2150nM). The response level at the steady state binding is plotted versus the log of the PDK1 concentration. The estimated Kd was obtained by fitting the data to a sigmoid curve using Kaleidagraph software. Kd for wild type PDK1 was 642 – 131 nM, PDK1 [T148A] was 64 – 7 nM and PDK1 [K76A] was 1744 – 167 nM. No detectable binding of PDK1 to the non-phosphorylated S6K-HM peptide (SESANQVFLGFTYVAPSV₂ SEQ ID NO:105) was detected with wild type PDK1 or any of the mutants (data not shown).

C. Activation of the indicated forms of PDK1 by S6K-pHM and S6K-HM. PDK1 activity was measured using the peptide substrate (T308tide) in the presence of the indicated concentrations of S6K-pHM (closed circles) and S6K-HM (open circles) as described in the methods. Assays were performed in triplicate and similar results obtained in 2 separate experiments. The results are the average – SD for a single experiment.

25 5. Interactions of regulatory phosphates with the αC helix

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A. The PDK1 backbone is shown as a ribbon, with helix α C in the centre of the view. Key residues are shown as sticks. The sulphate ion and the phosphate on the activation loop are also shown. A sticks model of ATP is shown. Hydrogen bonds are shown as black dotted lines.

B. Alignment of the amino acid sequence forming part of the phosphate pocket on PDK1 with the equivalent region of the indicated AGC kinases. Identical residues are denoted by white letters on a black background and similar residues by gray boxes. Arrows indicate the residues corresponding to Lys 76, Arg131, Thr148 and Gln150 of PDK1 (SEQ ID NOs:12 and 144). The aligned amino acid sequences are as follows: PKBα (SEQ ID NOs: 13 and 145), S6K1 (SEQ ID NOs: 14 and 146), SGK1 (SEQ ID NOs: 15 and 147), and Rsk1 (SEQ ID NOs: 16 and 148).

10 **6. Essential dynamics**

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- **A.** Projection of all available PKA crystal structures (labelled dots) and the PDK1 structure (diamond) onto the first two eigenvectors (i.e. the ones with the two largest eigenvalues) calculated from the PKA structures.
- **B.** Graphic representation of the motion along the first eigenvector, generated by projecting two structures at -4 nm (black) and +4 nm (grey).

7. Alignment of AGC protein kinase family members.

The alligned amino acid sequences and their respective corresponding sequence identifier are as follows:

P70S6Kalpha (SEQ ID NO: 17), P70S6Kbeta (SEQ ID NO: 18), P90RSK1 (SEQ ID NO: 19), P90RSK2 (SEQ ID NO: 20), P90RSK3 (SEQ ID NO: 21), MSK1 (SEQ ID NO: 22), MSK2 (SEQ ID NO: 23), PKBalpha (SEQ ID NO: 24), PKBbeta (SEQ ID NO: 25), PKBgamma (SEQ ID NO: 26), PRK1 (SEQ ID NO: 27), PRK2 (SEQ ID NO: 28), SGK1 (SEQ ID NO: 29), SGK3 (SEQ ID NO: 30), SGK2 (SEQ ID NO: 31), PKCbeta (SEQ ID NO: 32), PKCbetaII (SEQ ID NO: 33), PKCalpha (SEQ ID NO: 34), PKCgamma (SEQ ID NO: 35), PKCzeta (SEQ ID NO: 36), PKCiota (SEQ ID NO: 37), PKCdelta (SEQ ID NO: 38), PKAgamma (SEQ ID NO: 39), and PDK1 (SEQ ID NO: 40).

8. Staurosporine and UCN-01 electron density.

The staurosporine and UCN-01 molecules are shown in a stick representation. Hydrogen bonding atoms (Table 4) are labelled according to [49]. The unbiased $|F_o|-|F_c|$, ϕ_{calc} maps are contoured at 2.5 σ .

5 9..Details of the inhibitor binding sites.

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The bridging water molecule is shown as a sphere. Hydrogen bonds are indicated by black dotted lines. Labelled residues hydrogen-bond the inhibitor molecules.

Example 1: High resolution crystal structure of the human PDK1 catalytic domain defines the regulatory phosphopeptide docking site

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) plays a key role in insulin/growth factor induced signalling pathways through phosphorylation of downstream AGC-kinases such as Protein Kinase B/Akt and p70 ribosomal S6 kinase (S6K1). Here we describe the 2.0 Å crystal structure of the PDK1 kinase domain in complex with ATP. The structure defines the hydrophobic pocket termed the 'PIF-pocket' which plays a key role in mediating the interaction and phosphorylation of certain substrates such as S6K1. In the PDK1 structure, this pocket is occupied by an extensive crystallographic contact with another molecule of PDK1, reminiscent of the interaction of Protein Kinase A with the hydrophobic motif at its C-terminus. Previous studies have shown that phosphorylation of S6K1 at its C-terminal PIF-pocket-interacting motif, promotes the binding of S6K1 with PDK1, suggesting that there may be a phosphate docking site located nearby the PIF-pocket. Interestingly, close to the PIFpocket on the PDK1 structure, there is an ordered sulphate ion, interacting tightly with four surrounding side chains. The roles of these residues were investigated through a combination of site directed mutagenesis and kinetic studies, the results of which suggest that this region of PDK1 does indeed

represent a phosphate dependent docking site. An analogous phosphate binding regulatory motif may participate in the activation of other AGC kinases.

Results & Discussion

5 Overall structure

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The structure of the catalytic domain of PDK1 was solved by molecular replacement and refined to an R-factor of 0.19 (Rfree=0.22). PDK1 assumes the classic bilobal kinase fold (Fig. 1) and is similar to the only other AGC kinase structure solved, that of PKA (RMSD of 1.0 Å on C α atoms with PDB entry 1STC [Prade et al., 1997]). The form of PDK1 that was crystallized comprised residues 51 to 359. The tip of the activation loop (residues 233-236) is disordered, as observed in other kinase structures [Johnson et al., 1996]. The N-terminus (residue 51-70), which is pointing into a large void generated by the crystallographic symmetry, is also disordered. In contrast, the N-terminal extension to the kinase domain of PKA assumes an amphipathic a -helix (termed α A-helix), and packs against the kinase core [Knighton et al., 1991]. The cluster of hydrophobic residues that mediates this interaction in PKA is not present in PDK1, suggesting that the N-terminus of PDK1 could have a different function from that of PKA. Interestingly, it has recently been shown that the N-terminus of PDK1 (residues 1-50) interacts with Ral guanine nucleotide exchange factors [Tian et al., 2002]. Thus, this region may assume a unique conformation in PDK1, which is not defined by the structure described here.

PDK1 was crystallised in the presence of ATP but in the absence of any divalent cations. In the early stages of the refinement well-defined density for the entire ATP molecule could be observed. ATP adopts a different conformation to that observed in other kinase-ATP complexes (Fig. 1).

Perhaps due to the absence of divalent cations, the generally observed kink between the β and γ phosphate caused by the interaction with such an ion, is not seen in the PDK1 structure.

It is known that PDK1 can phosphorylate itself on residue Ser 241 in the activation loop and that this phosphorylation is required for PDK1 activity [Alessi et al., 1997]. Indeed, we observed density for a phosphate attached to this residue (Fig. 1), and extensive interactions are observed between this phosphoserine and residues from the C-terminal lobe and αC-helix (Fig. 1).

The interaction between Ser241 and the C-terminal lobe is similar to the equivalent interactions in PKA but as discussed below the binding to the αC-helix differs.

The PIF-pocket

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As outlined in the introduction, PDK1 was postulated to possess a pocket (the 'PIF-pocket') in the small lobe of its catalytic domain, required for the binding of PDK1 to the hydrophobic motif of its substrates [Biondi et al., 2000]. The PDK1 structure described here indeed reveals such a pocket, and shows that it lies in a location similar to the FXXF (SEQ ID NO:1)-binding pocket in PKA (Fig. 2). PDK1 residues Lys115, Ile118, Ile119 on the αB helix (Fig. 2), Val124, Val127 on the αC helix and Leu155 on β -sheet 5 form an approximately 5 Å deep pocket. Previous work has shown that mutation of Leu 155 to Glu abolishes the ability of PDK1 to interact with a peptide that encompasses the hydrophobic motif of PRK2 (PIFtide) [Biondi et al., 2000] as well as with S6K1, SGK1, PKCζ and PRK2 [Balendran et al., 2000, Biondi et al., 2000]. In addition, mutation of Lys115, Ile119, Glu150, and Leu155 to alanine, reduced the affinity of PDK1 for PIFtide approximately 10-fold, but did not affect the ability to phosphorylate and

activate S6K1 and SGK1 [Biondi et al., 2001]. These results are in agreement with the crystal structure of the PIF-pocket, since Leu155 is located at the center and the other residues line the wall of the pocket (Fig. 2). Interestingly, in our structure, the PIF-pocket is occupied by helix αG of a symmetry related molecule (Fig. 2). Tyr288 and Phe291 make hydrophobic contacts in this pocket with almost all pocket-lining residues, remarkably reminiscent of the interactions of the phenylalanines in the FXXF motif in PKA and their hydrophobic docking site in the equivalent region of the kinase domain (Fig. 2). In addition, residues Glu287, Gln292, Ile295 and Lys296 on the symmetry related loop also form contacts with residues lining the PIF-pocket. In total, 244 ² Å of accessible surface is buried by this contact, suggesting this is a tight interaction. However, the significance of this interaction is not clear as an oligomerisation event for PDK1 has not been demonstrated in solution previously. Indeed both the isolated catalytic domain of PDK1 that was crystallised and full length PDK1 migrate in gel filtration chromatography as apparent monomeric species (data not shown).

The phosphate pocket

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As outlined in the introduction, substrates of PDK1, such as S6K1, interact with the PIF-pocket of PDK1 with higher affinity when they are phosphorylated at their hydrophobic motif. This suggested that a regulatory phosphate binding site may be located close to the PIF-pocket. During refinement of the PDK1 structure, it became clear that next to the PIF-pocket another small pocket was present, occupied by a tetrahedral oxyanion (Fig. 2). As 2.0 M of sulphate was present in the crystallisation conditions, this was assigned as a sulphate ion. The ion interacts with four residues lining the pocket, namely Lys76, Arg131, Thr148 and Gln150.

Because of its close proximity to the PIF-pocket (approximately 5Å) it is possible that this sulphate-occupied pocket could represent the binding site for the phosphate on the phosphopeptide. To investigate this further, we mutated Lys76, Arg131, Thr148 and Gln150 to Ala, in order to verify the contribution of each of these residues in enabling PDK1 to interact with a peptide encompassing the hydrophobic motif of S6K1, in which the residue equivalent to Thr412 was phosphorylated (termed S6K-pHM). A quantitative surface plasmon resonance based binding assay (Fig. 4A) showed that wild type PDK1 interacted with S6K-pHM, with a Kd of 0.6 uM with S6K-pHM but not detectably to the non-phosphorylated form of this peptide (S6K-HM). The PDK1[R131A] and PDK1[Q150A] mutants did not detectably interact with S6K-pHM in this assay (Fig. 4B), confirming that the interactions these residues make in the PDK1 structure are of key importance. The PDK1[K76A] mutant interacted with 3-fold lower affinity (Kd 1.7 µM) with S6K-pHM. The PDK1[T148A] mutant however possessed about 10-fold higher (Kd 0.06 µM) affinity for S6KpHM than wild type PDK1. Moreover, the dissociation of PDK1[T148A] from S6K-pHM is markedly slower than that of wild type PDK1 or PDK1[K76A] (Fig 4A). These findings are unexpected as Thr148 is within hydrogen bonding distance of the sulphate (Fig. 2), but indicate that this residue may play a role in enabling the dissociation of PDK1 from S6KpHM.

The binding of PDK1 to PIFtide stimulates up to 4-fold the rate at which PDK1 phosphorylates a small peptide that encompasses the activation loop motif of PKB (termed T308tide) [Biondi et al., 2000], indicating that occupancy of the PIF-pocket of PDK1 activates the enzyme. Similarly, the binding of a phosphopeptide corresponding to the hydrophobic motif of RSK stimulated PDK1 activity 6-fold [Frodin et al., 2000]. We have now also found that the binding of S6K-pHM to wild type PDK1 induces a

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maximal 5-fold activation, with a half maximal activation occurring at a concentration of approximately 50 µM S6K-pHM (Fig. 4C). We next assayed the specific activities of PDK1[K76A], PDK1[R131A], PDK1[T148A] and PDK1[Q150A] mutants in the absence and presence of increasing concentrations of S6K-pHM (Fig. 4C). The PDK1[K76A] possessed the same specific activity towards T308tide in the absence of S6K-pHM as wild type PDK1, but an approximately 3-fold higher concentration of S6K-pHM was required to half maximally activate PDK1[K76A], consistent with the reduced affinity of this form of PDK1 for S6K-pHM (Fig. 4A,B). The PDK1[R131A] mutant possessed a 3-fold higher specific activity towards Thr308tide in the absence of S6K-pHM (Fig. 4C), as has been observed previously with certain other PIF-pocket mutants of PDK1(PDK1[K115A] and PDK1[L155E]) [Biondi et al., 2000]. However, in accordance with the inability of PDK1[R131A] to bind S6KpHM in the Biacore assay (Fig. 4B), it was not significantly activated by concentrations of S6K-pHM below 0.1 mM and its activity was only moderately further increased by the addition of high concentrations (0.3 and 1 mM) of S6K-pHM (Fig. 4C). The activity of a mutant of PDK1 in which both Lys76 and Arg131 were changed to Ala was activated even less significantly by these high concentrations of S6K-pHM. The PDK1[T148A] and PDK1[Q150A] mutants possessed similar specific activity towards T308tide as wild type PDK1 in the absence of S6K-pHM. The PDK1[T148A] mutant was activated similarly as wild type PDK1 by S6KpHM and consistent with the inability of PDK1[Q150A] to interact with S6K-pHM, this mutant of PDK1 was not significantly activated by concentrations of S6K-pHM below 0.1 mM but at 0.3 and 1 mM peptide a 2-3 fold activation was observed (Fig. 4).

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At very high peptide concentrations (0.3-1 mM) the non-phosphorylated S6K-HM

peptide induced a small (<2-fold) activation of PDK1 (Fig. 4C). Interestingly, despite the PDK1[K76A] and PDK1[R131A] mutants being markedly less able to interact with the phosphorylated S6K-pHM peptide, than wild type PDK1, high concentrations of the S6K-HM peptide activated PDK1[K76A] and PDK1[R131A] to a similar extent as wild type PDK1, indicating that the ability of these mutants to interact weakly with the S6K-HM peptide was not affected.

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We evaluated the sequence conservation in the phosphate pocket of the insulin/growth factor-activated AGC family kinases (PKBα, S6K1, SGK1 and RSK1). Sequence alignments indicate that this pocket is conserved amongst these kinases (Fig 5A). The most conserved residue is Gln150 which is found in all of these AGC kinases and the residue equivalent to Lys76 is always a basic residue (Fig. 5A). Arg131 is conserved in S6K1, SGK1 and RSK1 but not in PKBα, or PKBβ or PKBγ, where it is an Asn or Ser. Thr148 is conserved in PKBα and SGK1 but is an Ala in S6K1 and RSK1. Interestingly, we have found the Thr 148Ala mutation in PDK1 did not disrupt the phosphate pocket (Fig 4). As PKBα, S6K1, SGK1 and RSK1 require to be phosphorvlated at their hydrophobic motif to be maximally activated, it is tempting to speculate that the C-terminal hydrophobic motifs of these enzymes, when phosphorylated, bind to their own PIF/phosphate pockets, thereby generating a network of interactions similar to that of PDK1. In support of this, PKBα, S6K1, SGK1 and RSK1 also require phosphorylation of their activation loop at the position equivalent to Ser241 for activity. Consistent with PKA not possessing a phosphate pocket, Lys76 and Gln150 are not conserved in PKA (Fig. 3), and indeed such a pocket is not observed in the PKA structure (Fig. 2).

The αC helix

The PDK1 structure shows that, as in other protein kinases [Johnson et al., 2001, Husen and Kuriyan, 2002], the α C helix (residues 124-136) is a key signal integration motif in the kinase core. One turn of the PDK1 α C helix (residues 129-131, Figs. 3, 5) links together the N-terminal lobe, the C-terminal lobe and the active site. Arg129 points towards the activation loop and forms two hydrogen bonds with the phosphorylated Ser241, whereas Arg131 forms two hydrogen bonds with the sulphate in the phosphate pocket (Fig. 5). Glu130 coordinates Lys111 which forms a hydrogen bond with the α -phosphate of the bound ATP. This interaction is conserved in all protein kinases and shown to be crucial for activation [Johnson et al., 2001, Husen and Kuriyan, 2002]. An additional residue, His126, forms a third hydrogen bond with the phosphorylated Ser241. Val124 and Val127 on the α C helix are involved in formation of the PIF-pocket (Fig. 5).

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The αC helix provides a structural link between the putative phosphopeptide binding pocket and the phosphoserine in the activation loop. The fact that R131A has higher basal activity than wild type PDK1 may indicate that this residue plays tuning role in the PDK1 structure, not only participating in the activation of PDK1 in the presence of a phosphate ion, but also on keeping the equilibrium of the enzyme towards an inactive conformation in the absence of S6K-pHM. To our knowledge this is the first report of a kinase structure in which the αC helix is positioned by 2 regulatory phosphate binding sites on either side of the helix (Fig 5). This provides a possible sensor-mechanism for linking the phosphorylation-state of the activation loop and the phosphopeptide binding event in the PIF-pocket to PDK1 activity.

Activation state

All structures of PKA solved to date show a phosphorylated T-loop and are therefore assumed to be in an active state. In addition to the unphosphorylated versus phosphorylated states of PKA, there appear to be two main conformational states possible for the latter [Zheng et al., 1993, Johnson et al., 2001]. In the active, closed conformation, all residues are positioned to facilitate phosphoryl transfer. In contrast, the inactive, open conformation is seen in absence of a nucleotide, and differs from the closed conformation by conformational changes of the N-terminal and C-terminal domains with respect to each other. In addition, three 'intermediate' structures were described from PKA, having either adenosine (PDB entry 1BKX [Narayana et al., 1997]) or the inhibitors staurosporine (PDB entry 1STC [Prade et al., 1997]) and balanol (PDB entry 1BX6 [Narayana et al., 1999]) in the ATP-binding site. Taylor and colleagues have described a method to distinguish between the active and inactive conformations, based on three distances: His87-pThr197 (αC helix positioning), Ser53-Gly186 (opening of the glycine-rich loop) and Glu170-Tyr330 (C-terminal tail distance to active site) [Johnson et al., 2001]. In PDK1, only one of these distances, the opening state of the glycine rich loop, can be measured due to sequence conservation (Fig. 3). This distance is 12.4 Å, similar to a PKA intermediate conformation (this distance in PKA is 14.2Å for the open, 11.8 Å for intermediate and 10.0 Å for the closed conformation [Johnson et al., 2001]). To allow a more direct comparison of the PDK1 structure with the available PKA structures, we have analysed the conformational state of PDK1 in detail using a novel approach, which involves a principal component analysis (also called "essential dynamics" [Amadei et al.,1993]) of the crystallographic coordinates. In short, this involves the construction of a covariance matrix containing the correlations between atomic shifts (with respect to an average structure) in the ensemble of all available PKA crystal structures. Diagonalisation of this matrix gives eigenvector/eigenvalue sets which describe concerted shifts of atoms

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(eigenvectors) together with the corresponding mean square fluctuation of the structures (eigenvalues). This approach allows a condensed description of PKA conformational states using only a few degrees of freedom, as shown previously for a range of other proteins [van Aalten et al., 1997, van Aalten et al., 2000,deGroot et al., 1998]. Diagonalisation of a covariance matrix built from the backbone atoms of residues 37-196, 198-283 and 286-305 results in a set of eigenvectors that describe concerted motions of the PKA backbone. In Fig. 6A, all PKA structures are projected on a subspace spanned by the first two eigenvectors (i.e. those with the two largest eigenvalues). It appears that the PKA structures cluster in three main areas along the first eigenvector. On the left of the average structure (which by definition has a projection of 0.0 on all eigenvectors) are the structures that are known to be in the "open" conformation (Fig. 6A). Around the average structure lie the structures that have been shown to be in an "intermediate" conformation (complexes with the inhibitors staurosporine, balanol and adenosine). More to the right of the average structure are the PKA structures that are known to be in the "closed" conformation. Thus, we have captured the conformational state of PKA in a single variable, the translation along the first eigenvector. This is further clarified by investigation of the atomic shifts described by this eigenvector in Cartesian space (Fig. 6B). A hinge-bending motion is observed between the Nterminal and C-terminal lobes, opening and closing the active site. It is now possible directly to compare the PDK1 conformational state by projecting the structure (backbone atoms only) onto the PKA eigenvectors. Fig. 6A shows that the conformation of PDK1 is close to the PKA structures that are in an "intermediate" conformation, consistent with the other structural analyses described above.

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Conclusions

We have reported the structure of the PDK1 catalytic domain, which, although similar to PKA, has revealed important features that increase our understanding of the mechanism by which PDK1 is regulated. The structure, together with mutational analyses, defines a phosphopeptide binding pocket, consisting of a separate hydrophobic PIF-pocket and a phosphate binding site, which mediates the interaction of PDK1 with the phosphorylated hydrophobic motif of S6K. This is consistent with the previous hypothesis that phosphorylation of S6K and SGK [Biondi et al., 2001] as well as RSK [Frodin et al., 2000] at their FXXFS/T hydrophobic motif (SEQ ID NO:2) is the trigger for their interaction and phosphorylation by PDK1. In this mechanism the PIF-pocket would physiologically only interact with the Phe residues when the Ser/Thr residue is phosphorylated. Furthermore, as the phosphate pocket is conserved in other AGC kinases, the structural features and network of interaction of the phosphate pocket with the αC-helix on PDK1, could provide insight into the mode of activation of other AGC kinases.

Experimental Procedures

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Mammalian and Insect cells culture reagents were from Life Technologies. SensorChips SA were from BiaCore AB. Glutathione Sepharose, as well as pre- packed HiTrap Q HP and Hiload Superdex 200 prep grade columns were from Amersham Biosciences. Dialysis cassettes were from the Slide-A-Lyzer series (Pierce). Ni-NTA Agarose was from Qiagen. Disposable ultrafiltration devices (polyethersulfone membranes) were from Vivascience. Crystallisation research tools (primary screens, additive

screens and crystallisation plates) were from Hampton Research. Peptides were synthesised by Dr G. Blomberg (University of Bristol, UK).

General methods

Molecular biology techniques were performed using standard protocols. Site directed mutagenesis was performed using a QuickChange kit (Stratagene) following instructions provided by the manufacturer. DNA constructs used for transfection were purified from bacteria using Qiagen plasmid Mega kit according to the manufacturer's protocol, and their sequence verified. Human kidney embryonic 293 cells were cultured on 10 cm diameter dishes in Dulbecco's modified Eagle's medium containing 10% foetal bovine serum.

Buffers

Low Salt Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl; High Salt Buffer: 25mM Tris-HCl pH 7.5, 500 mM NaCl. Lysis Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl 0.07% β -mercaptoethanol, 1mM Benzamidine, and 20 μg/ml PMSF. Buffer A: 50 mM Tris-HCl pH 7.5, 1 mM EGTA, 1 mM EDTA, 1% (by mass) Triton-X 100, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 5 mM sodium pyrophosphate, 0.27 M sucrose, 1 μM microcystin-LR, 0.1% (by vol) β -mercaptoethanol and "complete" proteinase inhibitor cocktail (one tablet per 50 ml, Roche). Buffer B: 50 mM Tris/HCl pH 7.5, 0.1 mM EGTA, 10 mM β -mercaptoethanol and 0.27 M sucrose.

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A cDNA encoding for human PDK1 amino acid residues 51-359 with a stop codon inserted at position 360, was amplified by PCR reaction using full length human PDK1 cDNA in the pCMV5 vector [Alessi et al., 1997] as a template a 5'primer, which incorporates a BamH1 restriction site, an initiating methionine, a hexahistidine tag followed by a PreScission protease recognition sequence prior to the residue equivalent to Met51 of PDK1 (ggatcctataaatatggcacatcatcatcatcatcatctggaagttctgttccaggggcccatggacggcact gcagccgagcctcgg) (SEQ ID NO:106) and the 3' primer applied in this reaction was: 5'-ggatcctcaggtgagcttcggaggcgtctgctggtg-3' (SEQ ID NO: 107). The resulting PCR product was ligated into pCR 2.1 TOPO vector (Invitrogen) and then subcloned as a BamH1-BamH1 fragment into pFastbac1 vector (Life Technologies) for baculovirus protein expression. The resulting construct was then used to generate recombinant baculovirus using the Bac-to-Bac system (Life Technologies) following the manufacturer's protocol. The resulting baculoviruses were used to infect Sf21 cells at 1.5 x 106/ml. The infected cells were harvested by centrifugation 72 hours post infection. Cell pellets corresponding to 7 l of culture were resuspended in 900 ml of Lysis Buffer and cells lysed in nitrogen cavitation chamber. Cell debris was then pelleted by centrifugation, the supernatant made 0.5 M NaCl by addition of 4M NaCl and then incubated with Ni-NTA-Agarose (10 ml resin) for one hour. The resin was then washed in 10 times with 40 ml of Lysis Buffer containing 0.5M NaCl and then placed in a disposable Econo-Pac column (BioRad), where the resin was further washed with 700 ml of high salt buffer and then with 100 ml of low salt buffer, both supplemented with 10 mM imidazole. Elution was performed with 200 mM imidazole in high salt buffer and 2 ml fractions were collected. Fractions containing protein were pooled, diluted to 200 mM NaCl with 25 mM Tris/HCl pH 7.5, and loaded onto a 5 ml Hitrap Q sepharose column. The flow-through from this step, containing PDK1, was concentrated to 4 ml and then chromatographed on a 16/60

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Superdex 200 gel filtration column using an AKTA Explorer system (Amersham Biosciences) equilibrated with high salt buffer with the addition of 1mM DTT. PDK1 eluted in a large symmetric peak at the expected size for a monomer. The PDK1 containing peak was again pooled, concentrated and incubated with 300 µg GST-PreScission protease (expression construct kindly provided by John Heath, University of Birmingham, UK) on ice for 4h. In order to eliminate the cleaved His-tag sequences as well as any remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 µl glutathione-Sepharose and 200 µl Ni-NTA agarose resin for 15 minutes and the PDK1 protein that did not bind was collected. The resulting protein consists of PDK1 (51-359) preceded by a Gly-Pro at the N-terminus. The protein at this stage of the purification was apparently homogeneous as revealed by a single band after electrophoresis of 20 µg of protein on SDS-PAGE and staining with Coomasie Brilliant Blue R250 (data not shown).

Electrospray mass spectrometry revealed a main peak mass close to the expected size of this fragment of PDK1. The specific activity of PDK1 (51-359) towards the peptide T308tide and its activation in the presence of PIFtide was identical to wild type full length PDK1 [Biondi et al., 2000], and tryptic peptide mass finger printing indicated that PDK1 was quantitatively phosphorylated at Ser241 (data not shown). In BiaCore experiments, the steady state binding of PDK1 (51-359) to the peptide PIFtide was similar to that of the His-tag PDK1 (51-556) protein characterised previously [Balendran et al., 1999a].

Crystallisation and data collection

The PDK1 (51-359) protein was concentrated to a final concentration of 8.5 mg/ml (as determined by a Bradford assay using bovine serum albumin as a standard). The sitting drop vapour diffusion method was used for producing crystals. Sitting drops were formed by mixing 1 μl of protein solution with 1 μl of a mother liquor solution (0.1 M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP) with the addition of 0.2 μl EDTA (100mM). Hexagonal crystals (Table I) of PDK1 were grown at 20° C from a mother liquor containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP). Crystals appeared after one day, growing to 0.05 x 0.05 x 0.2 mm over 20 days. Crystals were frozen in a nitrogen gas stream after being soaked in 0.075 M Tris 8.5, 1.5M ammonium sulphate, 25% (v/v) glycerol.

Expression and purification of wild type and mutant forms of GST-PDK1.

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Wild type-PDK1 [Alessi et al., 1997], PDK1[R76A], PDK1[R131A], 15 PDK1[R76A,R131A], PDK1[T148A] and PDK1[Q150A] in the pEBG2T vector were used to express the wild type and indicated mutants of PDK1 fused through their N-terminus to glutathione S-transferase (GST). The GST fusion proteins were expressed in human embryonic kidney 293 cells. For the expression of each construct, twenty 10 cm diameter dishes of 293 20 cells were cultured and each dish transfected with 10 µg of the pEBG-2T construct, using a modified calcium phosphate method. 36 h posttransfection, the cells were lysed in 0.6 ml of ice-cold Buffer A, the lysates pooled, centrifuged at 4 ° C for 10 min at 13000 g and the GST-fusion 25 proteins were purified by affinity chromatography on glutathione-Sepharose and eluted in Buffer B supplemented with 20 mM glutathione as described previously [Alessi et al., 1997]. Typically between 1 and 2mg of each GST-fusion protein was obtained and each protein was more than 75 judged by SDS polyacrylamide gel electrophoresis (data not shown).

PDK1 catalytic activity measurements

The ability of wild type and mutant PDK1 to phosphorylate the synthetic peptide T308tide (KTFCGTPEYLAPEVRR ([Biondi et al., 2000]) (SEQ ID NO:108) was carried out in 30 µl assays containing 100 ng of wild type or mutant PDK1, 50 mM Tris/HCl pH 7.5, 0.1% β -mercaptoethanol, 10 mM MgCl₂, 100 μM [32γ P]ATP (200 cpm/pmol), 0.5 μM microcystin-LR, 1 mM T308tide in the presence or absence of the indicated concentrations of the S6K-pHM peptide (SESANQVFLGFT(P)YVAPSV) (SEQ ID NO:104) or S6K-HM.peptide (SESANQVFLGFTYVAPSV) (SEQ ID NO:105). After incubation for 10 min at 30 °C, 25 µl of the resultant mixture was spotted into P81 phosphocellulose paper (2 x 2 cm) and the papers washed and analysed as described previously for assays of MAP kinase. Control assays were carried out in parallel in which either PDK1, or peptide substrate were omitted; these values were always less than 5% of the activity measured in the presence of these reagents. One Unit of PDK1 activity was defined as that amount required to catalyse the phosphorylation of 1 nmol of the T308tide in 1 min.

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Biacore analysis

Binding was analysed in a BiaCore 3000 system (BiaCore AB, Stevenage, UK). Biotinylated S6K-pHM (Biotin-C₁₂- SESANQVFLGFT(P)YVAPSV) (SEQ ID NO:104) or the non-phosphorylated form of this peptide S6K-HM was bound to an streptavidin- coated Sensor chip (SA) (12 response units, RU). 30 μl of wild type or the indicated mutant GST-PDK1 were injected at a flow rate of 30μl/min, in buffer HBS-P (10 mM HEPES pH 7.4, 0.15M

NaCl, 0.005% (by vol) polysorbate-20) supplemented with 1 mM DTT. Specific interactions between S6K-pHM and PDK1 proteins were obtained between the concentration range of 2-2150 nM PDK1. Steady state binding was determined at each concentration. Dissociation of PDK1 from the phospho-peptide was monitored over a 1min period. Regeneration of the sensor chip surface was performed with 10µl injections of 0.05% SDS. As previously found for PDK1 binding to PIFtide [Biondi et al., 2000], the interaction data obtained using BiaCore did not fit to simple 1:1 interaction model. Apparent Kd values were estimated from the concentration of PDK1 which gives 50% of maximal response, which was obtained empirically using GST- PDK1[T148A] (RUmax=435). For all PDK1 construct tested, the off rates for S6Kp-HM were high in comparison to those of PIFtide binding with the time taken for 50% dissociation to occur for S6K-pHM is 30s compared to 1000s for PIFtide. This could account for the overall approximately 100-fold lower affinity of wild type PDK1 for S6K-pHM in comparison to PIFtide.

Data collection, structure solution, and refinement

Data on PDK1 crystals were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH1, using an ADSC Q4 CCD detector. The temperature of the crystals was maintained at 100K using a nitrogen cryostream. Data were processed using the HKL package [Otwinowski and Minor, 1997], statistics are shown in Table I.

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The structure of PDK1 was solved by molecular replacement with AMoRe [Navaza, 1994] using the structure of PKA in complex with an inhibitory peptide as a search model (PDB entry 1YDB), against 8-4 Ådata. A single, well separated solution was found with an R-factor of 0.479 (correlation

coefficient = 0.428). The structure was automatically built using warpNtrace [Perrakis et al., 1999], which found 262 of a possible 309 residues, giving an initial protein model with R=0.293 (Rfree=0.318) after simulated annealing in CNS [Brunger et al., 1998]. Iterative protein building in O [Jones et al., 1991] together with refinement in CNS, which included incorporation of a model for ATP, the phosphoserine in the activation loop, solvent molecules and a key sulphate molecule, resulted in a final model with R=0.195 (Rfree=0.222). No electron density was observed for residues 51-70 (the N-terminus of the construct) and 233-236 (the tip of the activation loop). All figures were made with PyMOL (http://www.pymol.org).

Table I

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Details of data collection & structure refinement for the PDK1 kinase domain. Values between brackets are for the highest resolution shell. All measured data were included in structure refinement.

	Wave length ()	0.933
	Space group	P3 ₂ 21
20	Unit cell ()	a=123.01, b=123.01, c=47.62
	Resolution ()	25-2.0 (2.07-1.0)
	Observed reflections	77315
	Unique reflections	27643
	Redundancy	2.8 (2.5)
25	Completeness(%)	98.0 (93.5)
	Rmerge	0.091 (0.454)
	I/ sigma I	7.3 (2.0)
	R _{free} reflections	579
	R _{cryst}	0.195

	R_{free}	0.222
	Number of groups	
	°°Protein residues	71-359
	°°Water	200
5	ATP	1
	SO ₄	5
	Glycerol	8
	Wilson B (²)	22.4
	< B > Protein	25.6
10	Water	35.7
	< B > ATP	38.8
	RMSD from ideal geometry	
	Bond lengths ()	0.005
	Bond angles (°)	1.34
15	Main chain B (²)	1.5.

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Example 2: Co-ordinates for PDK1 fragment with all alternate side chains.

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REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free r= 0.2220
    REMARK final r=0.1954 free r=0.2224
    REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0 REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
    REMARK rweight= 0.0900 (with wa= 1.29263)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /ddl/david/projects/PDK1_new/CNS/prot.par
REMARK parameter file 2 : /ddl/david/projects/PDK1_new/CNS/atp.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
    REMARK parameter file 4 : CNS_TOPPAR:ion.param

REMARK parameter file 5 : /ddl/david/projects/PDK1_new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
   REMARK B11= -2.766 B22= -2.766 B33= 5.532
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    REMARK B12= -0.375 B13=
                                 0.000 B23=
                                              0.000
    REMARK B-factor correction applied to coordinate array B: 0.031
    REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range:
                                                                     28210 ( 100.0
    웅 )
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                                       568 (
                                                                               2.0
    용 )
35
    REMARK number of reflections rejected:
                                                                         0 (
                                                                               0.0
    REMARK total number of reflections used:
                                                                     27642 (
                                                                              98.0
    REMARK number of reflections in working set:
                                                                     27063 ( 95.9
    REMARK number of reflections in test set:
                                                                       579 (
                                                                               2.1
    용 )
    CRYST1 123.013 123.013 47.624 90.00 90.00 120.00 P 32 2 1
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE:16-Apr-2002 18:31:12
                                            created by user: david
    REMARK VERSION: 1.0
    MOTA
              1 CB PRO A 71
                                  58.912 -7.251
                                                    8.216 1.00 67.78
    MOTA
              2 CG PRO A 71
                                 59.621 -6.941
                                                    9.534 1.00 69.16 A
    ATOM
              3 C PRO A 71
                                 59.493 -6.506 5.894 1.00 67.06 A
              4 O PRO A 71
    ATOM
                                 59.196 -5.318 5.766 1.00 66.66 A
              5 N PRO A 71
                                 60.984 -6.073 7.833 1.00 67.86 A
    MOTA
    MOTA
              6 CD PRO A 71
                                  60.554 -5.762
                                                   9.207 1.00 68.24 A
              7 CA PRO A 71
                                  60.040 -7.035 7.217 1.00 67.75 A
    АТОМ
              8 N PRO A 72
                                  59.356 -7.385 4.890 1.00 66.32 A
    MOTA
              9 CD PRO A 72
                                  59.712 -8.816 4.898 1.00 67.17 A
    ATOM
              10 CA PRO A 72
                                  58.840 -6.986 3.578 1.00 65.61 A
    MOTA
             11 CB PRO A 72
                                 58.672 -8.321 2.858 1.00 66.47 A
    MOTA
             12 CG PRO A 72
                                 59.796 -9.133 3.419 1.00 67.57 A
    ATOM
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	MOTA	13	С	PRO A		57.527	-6.208	3.673	1.00 63.94	Α
	ATOM	14	0	PRO A	72	56.710	-6.451	4.561	1.00 64.11	Α
	MOTA	15	N	ALA A	73	57.341	-5.268	2.753	1.00 61.57	A
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708	1.00 58.74	A
5	ATOM	17	СВ	ALA A	73	56.438	-3.030	3.165	1.00 58.05	A
	ATOM	18	С	ALA A		55.626	-4.448	1.271		Α
	ATOM	19	0	ALA A		56.347	-4.834	0.349		A
	ATOM	20	N	PRO A		54.372	-4.024	1.057		A
	ATOM	21	CD	PRO A		53.335	-3.610	2.018		A
10	ATOM	22	CA	PRO A		53.856	-4.003	-0.314		A
10	ATOM	23	CB	PRO A		52.474	-3.375	-0.148		
							-3.373			A
	ATOM	24	CG	PRO A		52.067		1.226		A
	ATOM	25	С	PRO A		54.772	-3.167	-1.204		A
1.7	ATOM	26	0	PRO A		55.559	-2.361	-0.708		A
15	ATOM	27	N	ALA A		54.680	-3.366	-2.514		A
	ATOM	28	CA	ALA A		55.503	-2.602	-3.446		A
	ATOM	29	СВ	ALA A	75	55.312	-3.121	-4.870	1.00 46.14	Α
	MOTA	30	С	ALA A	75	55.100	-1.134	-3.371		A
	ATOM	31	0	ALA A	75	53.947	-0.813	-3.086	1.00 41.01	А
20	ATOM	32	N	LYS A	76	56.053	-0.245	-3.619	1.00 38.31	Α
	ATOM	33	CA	LYS A	76	55.781	1.184	-3.588	1.00 35.72	A
	ATOM	34	СВ	LYS A	76	57.053	1.957	-3.930	1.00 37.70	Α
	ATOM	35	CG	LYS A	76	57.123	3.356	-3.350	1.00 40.99	A
	ATOM	36	CD	LYS A	76	57.262	3.316	-1.836	1.00 40.04	А
25	ATOM	37	CE	LYS A		57.511	4.705	-1.277		Α
	ATOM	38	NZ	LYS A		57.681	4.695	0.202		A
	ATOM	39	C	LYS A		54.708	1.467	-4.638		A
	ATOM	40	0	LYS A		54.814	1.005	-5.770		A
	ATOM	41	N	LYS A		53.668	2.207	-4.270		A
30	ATOM	42	CA	LYS A		52.619	2.517	-5.232		A
30	ATOM	43	CB	LYS A		51.316	2.865	-4.509		A
	ATOM	44	CG	LYS A		50.796	1.731	-3.631		
		45				49.487				A
	ATOM		CD	LYS A			2.089	-2.967		A
25	ATOM	46	CE	LYS A		49.136	1.091	-1.870		A
35	ATOM	47	NZ	LYS A		48.998	-0.296	-2.380		A
	ATOM	48	C	LYS A		53.053	3.668	-6.137		A
	ATOM	49	0	LYS A		54.010	4.377	-5.829		A
	ATOM	50	N	ARG A		52.351	3.838	-7.254		A
	ATOM	51	CA	ARG A		52.662	4.897	-8.211		A
40	ATOM	52	СВ	ARG A		53.574	4.344	-9.318		A
	ATOM	53	CG	ARG A		53.017		-10.050		А
	MOTA	54	CD	ARG A	78	54.092		-10.896		A
	MOTA	55	NE	ARG A	78	53.560	1.364	-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG A	78	52.985	0.270	-11.203	1.00 52.58	Α
45	ATOM	57	NH1	ARG A	78	52.860	0.113	-9.889	1.00 54.60	Α
	ATOM	58	NH2	ARG A	78	52.530	-0.672	-12.022	1.00 54.09	Α
	ATOM	59	С	ARG A	78	51.382	5.488	-8.803	1.00 23.76	A
	ATOM	60	0	ARG A	78	50.311	4.888	-8.706	1.00 24.25	Α
	ATOM	61	N	PRO A	79	51.475	6.676	-9.428	1.00 21.76	А
50	ATOM	62	CD	PRO A		52.691	7.475	-9.668		А
	ATOM	63	CA	PRO A		50.301		-10.021		А
	ATOM	64	СВ	PRO A		50.910		-10.816		A
	ATOM	65	CG	PRO A		52.124		-10.014		A
	ATOM	66	C	PRO A		49.446		-10.014		A
55	ATOM	67	0	PRO A		48.213		-10.903		
טט										A 7
	ATOM	68 60	N	GLU A		50.103		-11.714		A
	ATOM	69 70	CA	GLU A				-12.628		A
	ATOM	70	CB	GLU		50.393	3.994 -1			AC1
	ATOM	71	CG	GLU	80	51.230	2.907 -1	LZ.925	0.50 28.75 A	AC1

```
72
                             80 52.157
    MOTA
                 CD GLU
                                          2.224 -13.913
                                                          0.50 31.99 AC1
              73
                  OE1 GLU
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                                          2.897 -14.433
                                                         0.50 34.34 AC1
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                                          1.015 -14.172
                                                         0.50 32.83 AC1
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              74
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              75
                  С
                      GLU A
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    MOTA
              76
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                      GLU A
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                             81
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                      ASP
                          Α
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                      ASP A
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                  OD1 ASP A
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                                                                        Α
              82
                  OD2 ASP A
                             81
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                                                                               Α
    MOTA
              83
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                      ASP A
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              84
                  0
                      ASP A
                             81
                                                                               Α
              85
                             82
                                      46.445
                                               4.258
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                      PHE A
                                                                               Α
                             82
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                  CA
                      PHE A
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              87
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                  СВ
                      PHE A
                             82
                                                                               Α
    MOTA
              88
                  CG
                      PHE A
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                                      46.134
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20
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                                                                               Α
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                      PHE A
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                                                                               Α
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                                      43.182
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                                                              1.00 19.80
25
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                  N
                      LYS A
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                                                                               Α
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                  CA
                                      42.321
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                                                              1.00 21.65
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                                                                               Α
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                      LYS A
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                                                                               Α
              99
                      LYS A
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30
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                      PHE A
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                      PHE A
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                                                               1.00 17.68
                                                                               Α
    MOTA
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                  CD1 PHE A
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                                                                               Α
    MOTA
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                                                               1.00 19.66
                                                                               Α
    MOTA
             111
                  CE1 PHE A
                             84
                                      46.676
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                                                      -9.589
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                                                                               Α
             112
                  CE2 PHE A
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                                              10.816
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    ATOM
                                                                               Α
                                      46.936
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                                                               1.00 17.33
    ATOM
             113
                  CZ
                      PHE A
                             84
                                                                               Α
    ATOM
             114
                  С
                      PHE A
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                                      40.834
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                                                               1.00 20.72
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                      GLY A
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                                                               1.00 16.80
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                                      38.872
                                              11.810
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    MOTA
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                  CA
                      GLY A
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                                                               1.00 17.73
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                                                               1.00 18.75
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                      GLY A
                             85
                                      39.740
                                              14.043
                                                      -9.650
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    MOTA
             120
                  Ν
                      LYS A
                             86
                                      37.753
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                                                                               Α
             121
                      LYS A
                                      37.571
                                              15.064
                                                      -8.278
                                                              1.00 18.26
    ATOM
                  CA
                             86
                                                                               Α
                                                      -7.812
                                      36.133
                                              15.302
                                                              1.00 19.00
    MOTA
             122
                  СВ
                      LYS A
                             86
                                                                               Α
                  CG
                                      35.793
                                              14.660
                                                      -6.481
                                                               1.00 21.55
             123
                      LYS A
                             86
    MOTA
                                                                               Α
                                                      -6.066
             124
                  CD
                      LYS A
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                                                              1.00 26.48
    MOTA
                             86
                                                                               Α
                                      33.994
                                              14.239
                                                      -4.793
    MOTA
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                  CE
                      LYS A
                             86
                                                              1.00 31.92
                                                                               Α
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55
    ATOM
             126
                  NZ
                      LYS A
                             86
                                      32.568
                                              14.457
                                                              1.00 35.36
                                                                               Α
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    MOTA
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                      LYS A
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                                              15.571
                                                      -7.202
                                                              1.00 18.57
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                                                      -6.385
    MOTA
             128
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                      LYS A
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                                              14.807
                                                              1.00 16.77
                                                                               Α
                                                      -7.227
                                      38.737
             129
                  Ν
                      ILE A
                             87
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    ATOM
                                                                               Α
                                      39.577
                                             17.554 -6.256 1.00 18.26
    MOTA
             130
                 CA
                     ILE A 87
                                                                               Α
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	ATOM	131	СВ	ILE	Α	87	39.994	18.952	-6.772	1.00 19.60	A
	ATOM	132	CG2			87	40.593	19.786	-5.628	1.00 18.73	А
	MOTA	133	CG1	ILE	Α	87	40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134	CD1	ILE	Α	87	41.412	20.087	-8.588	1.00 25.26	A
5	ATOM	135	С	ILE	7\	87	38.731	17.709	-4.997	1.00 19.67	A
5											
	MOTA	136	0	ILE		87	37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU	Α	88	39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU	Δ	88	38.508	17.324	-2.611	1.00 20.68	A
						88	38.870			1.00 19.97	
	ATOM	139	СВ	LEU				16.151	-1.700		A
10	ATOM	140	CG	LEU	Α	88	38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141	CD1	LEU	Α	88	39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142	CD2	LEU	7\	88	37.029	14.622	-2.359	1.00 18.84	А
	ATOM	143	С	LEU		88	38.815	18.632	-1.901	1.00 23.11	A
	ATOM	144	0	LEU	Α	88	37.999	19.146	-1.139	1.00 25.10	A
15	ATOM	145	N	GLY	Α	89	39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY		89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	С	GLY	Α	89	41.658	20.954	-2.078	1.00 25.47	A
	MOTA	148	0	GLY	Α	89	42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU	Δ	90	41.870	22.254	-1.906	1.00 26.22	А
20											
20	ATOM	150	CA	GLU		90	43.064	22.924	-2.404	1.00 29.96	A
	MOTA	151	СВ	GLU	Α	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	Α	90	42.267	23.038	-4.831	1.00 34.32	A
	ATOM	153	CD	GLU		90	41.711	23.930	-5.927	1.00 38.27	А
	ATOM	154	OEI	GLU	А	90	40.590	24.456	-5.764	1.00 40.57	А
25	ATOM	155	OE2	GLU	Α	90	42.398	24.110	-6.952	1.00 40.90	A
	ATOM	156	С	GLU	Δ	90	43.711	23.768	-1.313	1.00 30.68	A
		157		GLU		90	43.049	24.574	-0.668	1.00 32.83	
	ATOM		0								A
	ATOM	158	N	GLY	Α	91	45.006	23.566	-1.104	1.00 29.66	A
	MOTA	159	CA	GLY	Α	91	45.724	24.332	-0.104	1.00 29.40	A
30	ATOM	160	С	GLY	Δ	91	46.795	25.151	-0.798	1.00 29.98	А
50											
	MOTA	161	0	GLY		91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER	Α	92	47.605	25.870	-0.029	1.00 28.30	A
	ATOM	163	CA	SER	Α	92	48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	СВ	SER		92	49.165	27.717	0.370	1.00 32.43	A
2.5											
35	ATOM	165	OG	SER	А	92	49.520	27.099	1.593	1.00 40.94	A
	ATOM	166	С	SER	Α	92	49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER	Δ	92	50.456	26.221	-2.143	1.00 30.46	A
	ATOM	168		PHE		93	50.087	24.703	-0.536	1.00 27.65	A
			N								
	MOTA	169	CA	PHE	Α	93	51.185	23.855	-0.995	1.00 26.34	A
40	ATOM	170	СВ	PHE	Α	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Δ	93	52.861	25.117	0.406	1.00 31.06	А
			CD1								
	ATOM	172				93	52.283	25.909	1.392	1.00 29.96	A
	MOTA	173	CD2	PHE	Α	93	53.949	25.613	-0.308	1.00 31.38	A
	MOTA	174	CE1	PHE	Α	93	52.779	27.181	1.665	1.00 32.69	A
45	ATOM	175		PHE		93	54.452	26.883	-0.044	1.00 32.63	А
15											
	MOTA	176	CZ	PHE		93	53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	С	PHE	Α	93	50.759	22.445	-1.365	1.00 25.39	A
	MOTA	178	0	PHE	Α	93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER		94	49.457	22.235	-1.519	1.00 23.63	A
50											
50	MOTA	180	CA	SER	А	94	48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER	Α	94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER		94	48.091	20.475	0.340	1.00 21.19	А
						94					
	ATOM	183	С	SER			47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER	Α	94	46.795	21.882	-2.173	1.00 18.76	A
55	MOTA	185	N	THR	Α	95	47.174	19.832	-3.038	1.00 19.38	A
	ATOM	186	CA	THR		95	45.840	19.637	-3.580	1.00 17.98	А
	ATOM	187	CB.	THR		95	45.818	19.818	-5.110	1.00 19.25	А
	MOTA	188	OG1	THR	Α	95	46.196	21.162	-5.434	1.00 22.04	A
	ATOM	189	CG2	THR	Α	95	44.421	19.549	-5.661	1.00 17.61	A
	==	-		`							

	ATOM	190	С	THR	Α	95	45.455	18.201	-3.243	1.00 1	.8.61	Α
	ATOM	191	0	THR	Ζ.	95	46.212	17.264	-3.524	1.00 1	7 10	A
	ATOM	192	N	VAL		96	44.295	18.024	-2.623	1.00 1		Α
	ATOM	193	CA	VAL	Α	96	43.845	16.685	-2.266	1.00 1	.6.05	Α
5	ATOM	194	СВ	VAL		96	43.170	16.672	-0.886	1.00 1		A
5												
	ATOM	195		VAL		96	42.741	15.249	-0.532	1.00 1	.8.02	Α
	ATOM	196	CG2	VAL	Α	96	44.145	17.206	0.168	1.00 1	.6.69	Α
	ATOM	197	С	VAL		96	42.875	16.207	-3.335	1.00 1		Α
	ATOM	198	0	VAL	Α	96	41.906	16.892	-3.665	1.00 1	.6.47	Α
10	ATOM	199	N	VAL	Α	97	43.157	15.033	-3.888	1.00 1	6.80	Α
	ATOM	200	CA	VAL		97	42.338	14.471	-4.949	1.00 1		Α
	MOTA	201	СВ	VAL	Α	97	43.153	14.354	-6.255	1.00 1	.8.43	Α
	ATOM	202	CG1	VAL	Δ	97	42.249	13.927	-7.404	1.00 1	9.69	Α
						97				1.00 1		
	ATOM	203		VAL			43.831	15.685	-6.569			A
15	ATOM	204	С	VAL	Α	97	41.812	13.091	-4.583	1.00 1	.6.77	Α
	ATOM	205	0	VAL	Ά	97	42.532	12.270	-4.014	1.00 1	7.13	Α
	ATOM	206	N	LEU		98	40.545	12.845	-4.895	1.00 1		A
	ATOM	207	CA	LEU	Α	98	39.947	11.548	-4.624	1.00 1	.7.04	Α
	ATOM	208	СВ	LEU	Δ	98	38.424	11.633	-4.743	1.00 1	6 89	Α
20												
20	ATOM	209	CG	LEU		98	37.635	10.342	-4.508	1.00 1		А
	ATOM	210	CD1	LEU	Α	98	37.990	9.762	-3.146	1.00 2	0.07	Α
	ATOM	211	CD2	LEU	Δ	98	36.143	10.627	-4.588	1.00 1		Α
	ATOM	212	С	LEU	А	98	40.512	10.597	-5.677	1.00 1		А
	ATOM	213	0	LEU	Α	98	40.527	10.920	-6.863	1.00 1	.8.60	Α
25	ATOM	214	N	ALA		99	40.995	9.438	-5.246	1.00 1		Α
23												
	ATOM	215	CA	ALA	А	99	41.570	8.466	-6.168	1.00 1	.8.42	Α
	ATOM	216	СВ	ALA	Α	99	43.090	8.524	-6.105	1.00 1	4.76	Α
	ATOM	217	С	ALA		99	41.102	7.055	-5.848	1.00 2		A
	ATOM	218	0	ALA	Α	99	40.941	6.691	-4.679	1.00 2	12.52	Α
30	ATOM	219	N	ARG	Α	100	40.878	6.261	-6.888	1.00 1	9.77	Α
				ARG				4.884				A
	MOTA	220	CA				40.459		-6.693	1.00 2		
	ATOM	221	СВ	ARG	Α	100	39.202	4.585	-7.518	1.00 2	4.22	Α
	ATOM	222	CG	ARG	Ά	100	38.608	3.205	-7.256	1.00 3	11.78	A
								2.979				
	ATOM	223	CD	ARG			37.326		-8.048	1.00 3		A
35	ATOM	224	NE	ARG	Α	100	36.213	3.818	-7.594	1.00 4	1.40	Α
	ATOM	225	CZ	ARG	A	100	35.566	3.662	-6.439	1.00 4	2.05	Α
		226		ARG			35.912	2.696	-5.598	1.00 4		
	ATOM											A
	ATOM	227	NH2	ARG	Α	100	34.559	4.468	-6.128	1.00 4	3.65	Α
	ATOM	228	С	ARG	Α	100	41.613	3.985	-7.129	1.00 1	8.63	Α
40	ATOM	229		ARG			42.078	4.065	-8.271	1.00 1		A
40			0									
	ATOM	230	N	GLU	Α	101	42.102	3.157	-6.212	1.00 1	.6.43	Α
	ATOM	231	CA	GLU	A	101	43.196	2.246	-6.533	1.00 1	6.11	A
	ATOM	232		GLU			43.774	1.637	-5.248	1.00 1		
			СВ									A
	ATOM	233	CG	GLU	А	101	44.917	0.657	-5.488	1.00 1	.6.51	Α
45	ATOM	234	CD	GLU	Α	101	45.501	0.115	-4.200	1.00 1	.8.20	Α
		235		GLU			44.733	-0.081	-3.239	1.00 1		
	ATOM											Α
	ATOM	236	OE2	GLU	Α	101	46.725	-0.132	-4.150	1.00 1	.7.14	Α
	ATOM	237	С	GLU	Α	101	42.625	1.152	-7.442	1.00 1	7.92	Α
	ATOM	238	0	GLU			41.681	0.462	-7.069	1.00 1		A
= 0												
50	ATOM	239	N	LEU	А	102	43.198	1.002	-8.632	1.00 1	.9.06	Α
	ATOM	240	CA	LEU	Α	102	42.718	0.025	-9.607	1.00 2	0.71	Α
	ATOM	241	СВ	LEU			43.569		-10.878	1.00 2		A
	ATOM	242	CG	LEU	Α	102	43.531	1.426	-11.642	1.00 2	15.30	Α
	ATOM	243	CD1	LEU	Α	102	44.577	1.414	-12.748	1.00 2	.7 . 88	Α
55	ATOM	244		LEU			42.140		-12.214	1.00 2		A
55												
	ATOM	245	С	LEU	Α	102	42.671	-1.418	-9.125	1.00 2	11.62	Α
	ATOM	246	0	LEU	Α	102	41.668	-2.103	-9.305	1.00 2	1.09	Α
		247	N	ALA			43.753	-1.874	-8.507	1.00 1		A
	ATOM											
	ATOM	248	CA	ALA	Α	T03	43.836	-3.249	-8.035	1.00 2	:U.87	Α

		_					_	_		
	MOTA	249	CB	ALA .	A 103	45.284	-3.571	-7.671	1.00 19.23	A
	ATOM	250	С	AT.A	A 103	42.919	-3.629	-6.872	1.00 19.92	A
									1.00 20.38	
	ATOM	251	0		A 103	42.703	-4.815	-6.628		A
	ATOM	252	N	THR .	A 104	42.361	-2.643	-6.175	1.00 18.12	A
5	ATOM	253	CA	THR .	A 104	41.517	-2.927	-5.018	1.00 17.15	A
	ATOM	254	СВ		A 104	42.212	-2.484	-3.717	1.00 19.54	A
	ATOM	255	OG1		A 104	42.456	-1.070	-3.773	1.00 19.26	A
	ATOM	256	CG2	THR .	A 104	43.536	-3.219	-3.529	1.00 17.02	A
	ATOM	257	С	THR .	A 104	40.159	-2.247	-5.026	1.00 19.44	A
10	ATOM	258	0		A 104	39.259	-2.648	-4.285	1.00 18.70	А
10										
	ATOM	259	N		A 105	40.034	-1.207	-5.847	1.00 19.65	A
	ATOM	260	CA	SER .	A 105	38.819	-0.400	-5.967	1.00 19.37	A
	ATOM	261	СВ	SER	105	37.598	-1.304	-6.173	0.50 21.81	AC1
	ATOM	262	OG	SER	105	36.431	-0.539	-6.412	0.50 23.01	AC1
1.5										
15	ATOM	263	С		A 105	38.644	0.447	-4.701	1.00 18.99	A
	ATOM	264	0	SER .	A 105	37.602	1.070	-4.488	1.00 18.66	A
	ATOM	265	N	ARG .	A 106	39.674	0.468	-3.861	1.00 16.84	A
	ATOM	266	CA		A 106	39.655	1.267	-2.634	1.00 16.21	А
	ATOM	267	СВ		A 106	40.827	0.886	-1.723	1.00 16.41	A
20	ATOM	268	CG	ARG .	A 106	40.619	-0.367	-0.906	1.00 15.49	A
	ATOM	269	CD	ARG .	A 106	41.887	-0.755	-0.170	1.00 17.43	A
	ATOM	270	NE		A 106	41.620	-1.792	0.824	1.00 20.47	A
						42.548				
	ATOM	271	CZ		A 106		-2.568	1.371	1.00 20.24	A
	ATOM	272	NH1	ARG .	A 106	43.821	-2.433	1.017	1.00 17.80	A
25	ATOM	273	NH2	ARG .	A 106	42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG	A 106	39.785	2.746	-2.981	1.00 17.37	A
								-3.902		
	ATOM	275	0		A 106	40.514	3.103		1.00 17.75	A
	ATOM	276	N	GLU .	A 107	39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU .	A 107	39.156	5.039	-2.461	1.00 20.80	A
30	ATOM	278	СВ	GLU	A 107	37.779	5.694	-2.337	1.00 22.93	A
	ATOM	279	CG		A 107	36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD		A 107	35.431	5.975	-3.148	1.00 32.40	A
	ATOM	281	OE1	GLU .	A 107	35.262	6.939	-3.923	1.00 33.74	A
	ATOM	282	OE2	GLU .	A 107	34.608	5.654	-2.263	1.00 36.00	A
35	ATOM	283	С		A 107	40.053	5.678	-1.410	1.00 18.93	A
33										
	ATOM	284	0		A 107	39.891	5.427	-0.220	1.00 19.21	A
	ATOM	285	N	TYR .	A 108	40.988	6.507	-1.852	1.00 16.70	A
	ATOM	286	CA	TYR .	A 108	41.883	7.209	-0.942	1.00 15.86	A
	ATOM	287	СВ	TYR	A 108	43.325	6.728	-1.104	1.00 15.30	A
40	ATOM	288	CG		A 108	43.593	5.328	-0.612	1.00 16.33	A
40										
	ATOM	289			A 108	43.765	5.066	0.746	1.00 16.36	A
	ATOM	290	CE1	TYR .	A 108	44.046	3.769	1.201	1.00 18.48	A
	ATOM	291	CD2	TYR .	A 108	43.701	4.268	-1.511	1.00 13.25	A
	ATOM	292			A 108	43.980	2.981	-1.075	1.00 17.28	A
15										
45	ATOM	293	CZ		A 108	44.152	2.736	0.276	1.00 19.17	A
	ATOM	294	OH	TYR .	A 108	44.440	1.461	0.688	1.00 19.38	A
	ATOM	295	С	TYR .	A 108	41.850	8.687	-1.292	1.00 16.80	A
	ATOM	296	0		A 108	41.560	9.058	-2.431	1.00 15.22	A
		297	N		A 109			-0.306	1.00 14.61	
50	ATOM					42.132	9.528			A
50	ATOM	298	CA		A 109	42.207	10.957	-0.539	1.00 14.30	A
	ATOM	299	СВ	ALA .	A 109	41.671	11.726	0.661	1.00 14.78	A
	ATOM	300	С	ALA .	A 109	43.713	11.136	-0.667	1.00 16.79	A
	ATOM	301	0		A 109	44.450	10.983	0.317	1.00 16.52	A
	ATOM	302	N		A 110	44.182	11.410	-1.881	1.00 14.80	A
55	ATOM	303	CA	ILE .	A 110	45.609	11.574	-2.093	1.00 15.80	A
	ATOM	304	СВ	ILE .	A 110	46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305			A 110	47.550	11.098	-3.632	1.00 16.80	A
	ATOM	306			A 110	45.774	9.358	-3.284	1.00 17.76	A
	ATOM	307	CD1	ILE .	A 110	46.308	8.513	-4.437	1.00 16.07	A

	ATOM	308	С	ILE .	A	110	46.004	13.045	-2.129	1.00	17.78	A
	ATOM	309	0	ILE .			45.534	13.813	-2.976	1.00	16.24	A
	ATOM	310	N	LYS .			46.846	13.435	-1.177		16.15	A
	ATOM	311	CA	LYS .			47.326	14.808	-1.100		17.20	A
5	ATOM	312		LYS .			47.700	15.176	0.344		17.41	
3			CB									A
	ATOM	313	CG	LYS .			48.350	16.547	0.464		20.71	A
	ATOM	314	CD	LYS .			48.585	16.971	1.910		24.25	A
	ATOM	315	CE	LYS .	A	111	47.288	17.381	2.598	1.00	29.46	A
	MOTA	316	NZ	LYS .	A	111	47.516	17.866	4.000	1.00	30.50	Α
10	ATOM	317	С	LYS .	Α	111	48.551	14.890	-1.994	1.00	16.41	Α
	ATOM	318	0	LYS .	Α	111	49.509	14.137	-1.813	1.00	18.20	Α
	ATOM	319	N	ILE .	Α	112	48.509	15.798	-2.963	1.00	15.87	Α
	ATOM	320	CA	ILE .	A	112	49.606	15.967	-3.907	1.00	17.28	A
	ATOM	321	СВ	ILE .			49.079	15.911	-5.358	1.00	16.43	А
15	ATOM	322		ILE .			50.235	15.998	-6.341		15.12	A
15	ATOM	323	CG1				48.293	14.609	-5.565		16.82	A
	ATOM	324		ILE .			47.580	14.511	-6.904		18.47	A
								17.301				
	ATOM	325	C	ILE .			50.307		-3.663		19.03	A
20	ATOM	326	0	ILE .			49.669	18.350	-3.635		19.15	A
20	ATOM	327	N	LEU .			51.622	17.245	-3.472		20.22	A
	ATOM	328	CA	LEU .			52.416	18.442	-3.214		22.36	A
	ATOM	329	СВ	LEU .	A	113	52.995	18.397	-1.794	1.00	22.13	Α
	ATOM	330	CG	LEU .	A	113	52.042	18.063	-0.646	1.00	22.46	Α
	ATOM	331	CD1	LEU .	Α	113	51.866	16.557	-0.553	1.00	23.81	Α
25	ATOM	332	CD2	LEU .	Α	113	52.603	18.595	0.660	1.00	23.68	Α
	ATOM	333	С	LEU .	A	113	53.560	18.547	-4.215	1.00	23.37	A
	ATOM	334	0	LEU .	Α	113	54.300	17.586	-4.424	1.00	23.11	A
	ATOM	335	N	GLU .			53.706	19.714	-4.834		23.88	A
	ATOM	336	CA	GLU .			54.771	19.920	-5.806		26.00	A
30	ATOM	337	CB	GLU .			54.435	21.111	-6.706		27.74	A
30	ATOM	338	CG	GLU .			55.533	21.452	-7.696		35.07	A
	ATOM	339	CD	GLU .			55.220	22.696	-8.497		39.24	A
	ATOM	340		GLU .			54.808	23.703	-7.885		41.45	A
	ATOM	341	OE2				55.395	22.670	-9.736		44.05	A
35	ATOM	342	С	GLU .			56.087	20.163	-5.067		24.37	A
	ATOM	343	0	GLU .			56.186	21.071	-4.238		24.43	A
	MOTA	344	N	LYS .	A	115	57.096	19.350	-5.360	1.00	24.10	Α
	ATOM	345	CA	LYS .	A	115	58.376	19.493	-4.678	1.00	24.93	Α
	ATOM	346	СВ	LYS .	A	115	59.339	18.373	-5.103	1.00	23.72	A
40	MOTA	347	CG	LYS .	Α	115	59.139	17.080	-4.308	1.00	23.09	Α
	ATOM	348	CD	LYS .	A	115	60.064	15.944	-4.743	1.00	21.92	A
	ATOM	349	CE	LYS .			59.691	15.400	-6.117	1.00	22.42	A
	ATOM	350	NΖ	LYS .			60.447	14.150	-6.448		19.71	A
	ATOM	351	C	LYS .			59.031	20.858	-4.868		26.87	A
45	ATOM	352	0	LYS .			59.492	21.469	-3.903		26.17	A
73							59.058		-6.102			
	ATOM	353	N	ARG .				21.348			28.73	A.
	ATOM	354	CA	ARG .	A		59.678	22.638	-6.380		29.66	A
	ATOM	355	СВ	ARG		116	59.533	22.980	-7.868		31.29	AC1
	ATOM	356	CG	ARG		116	60.047	24.361	-8.267		33.19	AC1
50	ATOM	357	CD	ARG		116	61.368	24.710	-7.590		35.13	AC1
	ATOM	358	NE	ARG		116	62.329	23.612	-7.618	0.50	36.42	AC1
	ATOM	359	CZ	ARG		116	63.510	23.648	-7.009	0.50	36.18	AC1
	ATOM	360	NH1	ARG		116	63.871	24.729	-6.332	0.50	36.12	AC1
	ATOM	361	NH2	ARG		116	64.324	22.602	-7.067		35.77	AC1
55	ATOM	362	С	ARG .	A		59.097	23.761	-5.519		29.70	А
	ATOM	363	0	ARG .			59.843	24.515	-4.889		29.16	A
	ATOM	364	N	HIS .			57.773	23.862	-5.472		27.22	A
	ATOM	365	CA	HIS .			57.126	24.903	-4.681		26.33	A
		366							-4.848			
	ATOM	200	СВ	HIS .	Н	тт /	55.606	24.835	-4.040	1.00	28.41	A

	ATOM	367	CG	HIS A 11	54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368		HIS A 11		27.249	-3.935	1.00 31.02	A
		369		HIS A 11			-3.961	1.00 33.13	
	ATOM								A
_	ATOM	370		HIS A 11		27.148	-3.480	1.00 34.58	A
5	ATOM	371		HIS A 11		27.940	-3.455	1.00 35.18	A
	ATOM	372	С	HIS A 11			-3.202	1.00 26.22	A
	ATOM	373	0	HIS A 11			-2.534	1.00 25.67	А
	ATOM	374	N	ILE A 118		23.554	-2.689	1.00 24.94	A
	MOTA	375	CA	ILE A 118	57.792	23.315	-1.285	1.00 23.94	A
10	ATOM	376	СВ	ILE A 118	57.711	21.812	-0.952	1.00 23.50	A
	ATOM	377	CG2	ILE A 118	58.374	21.533	0.389	1.00 23.76	A
	ATOM	378	CG1	ILE A 118	56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379	CD1	ILE A 118	56.066	19.858	-0.834	1.00 28.06	A
	ATOM	380	С	ILE A 118	59.195	23.821	-0.958	1.00 23.78	A
15	ATOM	381	0	ILE A 118	59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE A 119			-1.815	1.00 23.46	А
	ATOM	383	CA	ILE A 119		23.913	-1.619	1.00 25.13	А
	ATOM	384	СВ	ILE A 119			-2.664	1.00 24.25	A
	ATOM	385	CG2			23.890	-2.617	1.00 22.47	A
20	ATOM	386		ILE A 119		21.738	-2.395	1.00 25.05	A
20	ATOM	387		ILE A 119		20.945	-3.439	1.00 24.62	A
	ATOM	388	C	ILE A 119		25.435	-1.705	1.00 24.02	A
	ATOM	389	0	ILE A 119		26.051	-0.872	1.00 23.30	A
25	ATOM ATOM	390	N	LYS A 120		26.039 27.489	-2.704 -2.879	1.00 27.67	A
25		391	CA	LYS A 120				1.00 30.29	A
	ATOM	392	CB	LYS A 120		27.940	-4.060	1.00 32.34	A
	ATOM	393	CG	LYS A 120			-5.409	1.00 39.30	A
	ATOM	394	CD	LYS A 120		27.950	-6.512	1.00 45.19	A
•	ATOM	395	CE	LYS A 120		27.636	-6.218	1.00 46.48	A
30	ATOM	396	NZ	LYS A 120		28.155	-7.252	1.00 46.49	A
	ATOM	397	С	LYS A 120		28.247	-1.638	1.00 30.89	A
	ATOM	398	0	LYS A 120		29.198	-1.217	1.00 32.48	A
	ATOM	399	N	GLU A 121		27.825	-1.055	1.00 29.82	A
	MOTA	400	CA	GLU A 121	L 58.986	28.488	0.128	1.00 30.33	A
35	MOTA	401	CB	GLU A 121	L 57.455	28.416	0.117	1.00 33.04	A
	MOTA	402	CG	GLU A 121	L 56.794	29.021	-1.120	1.00 36.45	A
	ATOM	403	CD	GLU A 121	L 57.221	30.456	-1.373	1.00 39.88	A
	ATOM	404	OE1	GLU A 121	L 57.200	31.264	-0.420	1.00 40.53	A
	ATOM	405	OE2	GLU A 121	L 57.573	30.778	-2.529	1.00 43.24	A
40	ATOM	406	С	GLU A 121	L 59.511	27.930	1.451	1.00 30.37	A
	ATOM	407	0	GLU A 121	L 58.946	28.204	2.513	1.00 31.24	A
	ATOM	408	N	ASN A 122	60.588	27.151	1.390	1.00 29.03	A
	ATOM	409	CA	ASN A 122	61.183	26.573	2.594	1.00 28.46	A
	ATOM	410	СВ	ASN A 122		27.673	3.436	1.00 31.28	А
45	ATOM	411	CG	ASN A 122		28.395	2.698	1.00 34.12	A
	ATOM	412		ASN A 122		29.143	1.754	1.00 35.57	A
	ATOM	413		ASN A 122		28.169	3.127	1.00 35.73	A
	ATOM	414	C	ASN A 122		25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN A 122		26.055	4.663	1.00 27.23	A
50	ATOM	416	N	LYS A 123		24.955	2.842	1.00 23.99	A
30	ATOM	417	CA	LYS A 123		24.210	3.574	1.00 23.33	A
				LYS A 123		24.210	2.810		
	MOTA	418	CB					1.00 21.97	A
	MOTA	419	CG	LYS A 123		25.645	2.599	1.00 25.68	A
	ATOM	420	CD	LYS A 123		26.354	3.927	1.00 27.54	A
55	ATOM	421	CE	LYS A 123		27.796	3.716	1.00 31.30	A
	ATOM	422	NΖ	LYS A 123		28.540	5.004	1.00 33.21	A
	ATOM	423	C	LYS A 123		22.759	3.821	1.00 22.20	A
	ATOM	424	0	LYS A 123		21.960	4.264	1.00 22.50	A
	ATOM	425	N	VAL A 12	59.997	22.412	3.535	1.00 20.59	A

	ATOM	426	CA	VAL	Δ	124	60.439	21.039	3.730	1.00	20.25	А
	ATOM	427	СВ	VAL			61.922	20.850	3.328		19.43	A
	ATOM	428		VAL			62.346	19.407	3.573		18.69	A
	ATOM	429		VAL			62.104	21.195	1.853		18.21	A
_												
5	ATOM	430	С	VAL			60.236	20.561	5.163		19.53	A
	ATOM	431	0	VAL			59.841	19.418	5.385		20.02	A
	ATOM	432	N	PRO			60.513	21.422	6.159		20.01	A
	ATOM	433	CD	PRO			61.178	22.738	6.118	1.00	18.69	A
	ATOM	434	CA	PRO	Α	125	60.318	20.979	7.544	1.00	19.88	A
10	ATOM	435	СВ	PRO	Α	125	60.793	22.180	8.363	1.00	19.95	A
	ATOM	436	CG	PRO	Α	125	61.839	22.805	7.479	1.00	18.85	A
	ATOM	437	С	PRO	Α	125	58.848	20.642	7.824	1.00	19.76	А
	ATOM	438	0	PRO	Α	125	58.544	19.700	8.550	1.00	16.99	А
	ATOM	439	N	TYR			57.947	21.418	7.235		18.98	А
15	ATOM	440	CA	TYR			56.516	21.220	7.435		21.97	A
13	ATOM	441	CB	TYR			55.752	22.448	6.933		25.17	A
		442	CG	TYR			56.040	23.690	7.748		30.98	A
	ATOM											
	ATOM	443		TYR			55.438	23.886	8.991		33.95	A
• •	ATOM	444		TYR			55.721	25.015	9.763		36.60	A
20	ATOM	445		TYR			56.938	24.657	7.292		35.43	A
	ATOM	446	CE2	TYR			57.231	25.792	8.058		37.20	A
	ATOM	447	CZ	TYR	Α	126	56.618	25.962	9.291	1.00	37.40	A
	ATOM	448	OH	TYR	Α	126	56.903	27.073	10.052	1.00	40.85	A
	ATOM	449	С	TYR	Α	126	55.990	19.956	6.762	1.00	21.35	A
25	ATOM	450	0	TYR	Α	126	55.265	19.175	7.383	1.00	20.49	A
	ATOM	451	N	VAL	Α	127	56.354	19.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL	Α	127	55.892	18.562	4.790	1.00	17.58	А
	ATOM	453	СВ	VAL			56.308	18.596	3.308		17.45	A
	ATOM	454		VAL			55.786	17.350	2.600		17.97	A
30	ATOM	455		VAL			55.751	19.850	2.641		14.90	A
30		456		VAL							18.39	
	ATOM		C				56.459	17.306	5.448			A
	ATOM	457	0	VAL			55.769	16.298	5.583		18.14	A
	ATOM	458	N	THR			57.716	17.381	5.869		17.50	A
	ATOM	459	CA	THR			58.375	16.260	6.530		18.54	A
35	ATOM	460	СВ	THR	Α	128	59.861	16.586	6.805	1.00	18.01	A
	ATOM	461	OG1	THR	Α	128	60.537	16.804	5.559	1.00	21.14	A
	ATOM	462	CG2	THR	Α	128	60.536	15.446	7.545	1.00	17.95	A
	ATOM	463	С	THR	Α	128	57.676	15.941	7.856	1.00	19.49	A
	ATOM	464	0	THR	Α	128	57.438	14.776	8.179	1.00	18.76	А
40	ATOM	465	N	ARG			57.345	16.981	8.619	1.00	19.60	А
	ATOM	466	CA	ARG			56.673	16.804	9.904		20.12	A
	ATOM	467	СВ	ARG			56.534	18.144	10.621		21.33	A
	ATOM	468	CG	ARG			55.948	18.029	12.023		28.02	A
	ATOM	469	CD					19.404	12.523		31.25	
15				ARG			55.721					A
45	ATOM	470	NE	ARG			56.940	20.205	12.560		37.78	A
	ATOM	471	CZ	ARG			56.962	21.524	12.391		40.10	A
	ATOM	472		ARG			55.828	22.197	12.239		40.03	A
	ATOM	473	NH2	ARG			58.119	22.170	12.374	1.00	44.58	A
	ATOM	474	С	ARG	Α	129	55.288	16.186	9.729	1.00	20.08	A
50	ATOM	475	0	ARG	Α	129	54.891	15.305	10.496	1.00	20.40	A
	ATOM	476	N	GLU	Α	130	54.553	16.654	8.724	1.00	18.79	A
	ATOM	477	CA	GLU			53.222	16.125	8.454	1.00	20.10	A
	ATOM	478	СВ	GLU			52.638	16.749	7.183		19.92	А
	ATOM	479	CG	GLU			51.350	16.087	6.708		27.85	A
55	ATOM	480	CD	GLU			50.581	16.933	5.707		29.72	A
22	ATOM	481		GLU			51.216	17.528	4.814		33.46	A
				GLU								
	ATOM	482					49.339	16.996	5.807		30.74	A
	ATOM	483	C	GLU			53.301	14.615	8.295		19.81	A
	ATOM	484	0	GLU	А	T30	52.553	13.875	8.935	1.00	18.37	A

	ATOM	485	N	ARG	Α	131	54.219	14.162	7.447	1.00	20.41	A
	ATOM	486	CA	ARG	Δ	131	54.397	12.735	7.202	1 00	22.45	А
	ATOM	487	СВ	ARG			55.442	12.511	6.098		25.16	A
	ATOM	488	CG	ARG	Α	131	55.742	11.043	5.840	1.00	28.75	A
5	ATOM	489	CD	ARG	Ζ\	131	56.736	10.837	4.708	1 00	33.75	A
5												
	ATOM	490	NE	ARG			57.020	9.415	4.520		40.07	A
	ATOM	491	CZ	ARG	Α	131	57.756	8.915	3.532	1.00	43.07	A
	ATOM	492	NH1	ARG	Α	131	58.293	9.721	2.625	1.00	44.91	A
	ATOM	493		ARG			57.955	7.606	3.449		44.45	A
10												
10	ATOM	494	С	ARG			54.820	11.982	8.466		23.24	A
	ATOM	495	0	ARG	Α	131	54.241	10.948	8.804	1.00	23.86	A
	ATOM	496	N	ASP	Α	132	55.831	12.497	9.160	1.00	21.99	A
	ATOM	497	CA	ASP			56.318	11.850	10.370		22.04	A
	ATOM	498	СВ	ASP	Α	132	57.570	12.564	10.888		23.72	A
15	ATOM	499	CG	ASP	Α	132	58.750	12.442	9.932	1.00	27.77	A
	ATOM	500	OD1	ASP	Α	132	58.681	11.620	8.989	1.00	27.34	А
							59.753				28.70	
	ATOM	501		ASP				13.163	10.128			А
	ATOM	502	С	ASP	Α	132	55.258	11.772	11.474	1.00	21.69	A
	ATOM	503	0	ASP	Α	132	55.077	10.723	12.092	1.00	22.75	A
20	ATOM	504	N	VAL	Δ	133	54.551	12.868	11.725	1 00	19.54	А
20												
	ATOM	505	CA	VAL			53.525	12.843	12.759		18.52	A
	MOTA	506	СВ	VAL	Α	133	52.908	14.244	12.990	1.00	19.26	A
	ATOM	507	CG1	VAL	Α	133	51.708	14.135	13.918	1.00	18.79	A
	ATOM	508		VAL			53.953	15.180	13.604		18.80	A
2.5												
25	ATOM	509	С	VAL			52.419	11.854	12.398		19.46	A
	ATOM	510	0	VAL	Α	133	52.073	10.991	13.200	1.00	19.94	A
	ATOM	511	N	MET	Α	134	51.878	11.957	11.187	1.00	19.15	A
	ATOM	512		MET			50.807	11.052	10.792		21.25	A
			CA									
	ATOM	513	СВ	MET	Α	134	50.309	11.381	9.383	1.00	17.34	A
30	ATOM	514	CG	MET	Α	134	49.615	12.730	9.302	1.00	20.00	A
	ATOM	515	SD	MET	Δ	134	48.643	12.952	7.798	1 00	24.21	A
	ATOM	516	CE	MET			47.033	12.434	8.400		23.20	A
	ATOM	517	С	MET	Α	134	51.203	9.582	10.881	1.00	22.43	A
	ATOM	518	0	MET	Α	134	50.384	8.741	11.249	1.00	23.82	A
35	ATOM	519	N	SER	7\	135	52.454	9.273	10.556	1 00	23.09	А
33												
	ATOM	520	CA	SER			52.939	7.895	10.615		26.13	A
	ATOM	521	СВ	SER	Α	135	54.356	7.798	10.039	1.00	26.17	A
	ATOM	522	OG	SER	Α	135	54.383	8.177	8.673	1.00	31.91	A
	ATOM	523	С	SER			52.957	7.358	12.045		26.58	А
40												
40	ATOM	524	0	SER			52.926	6.148	12.261		26.42	А
	MOTA	525	N	ARG	Α	136	53.014	8.261	13.018	1.00	25.65	A
	ATOM	526	CA	ARG	Α	136	53.056	7.870	14.425	1.00	27.47	A
	ATOM	527	СВ	ARG			53.823	8.914	15.238		27.97	A
	ATOM	528	CG	ARG			55.283	9.082	14.857		32.00	A
45	MOTA	529	CD	ARG	Α	136	55.904	10.218	15.664	1.00	33.03	A
	ATOM	530	NE	ARG	Α	136	55.602	10.073	17.084	1.00	36.11	A
				ARG			55.867					
	ATOM	531	CZ					10.990	18.007		39.74	A
	ATOM	532	NHI	ARG	Α	136	56.449	12.132	17.661	1.00	40.55	A
	ATOM	533	NH2	ARG	Α	136	55.540	10.769	19.276	1.00	36.72	A
50	ATOM	534	С	ARG			51.667	7.709	15.036	1.00	26.38	А
•												
	ATOM	535	0	ARG			51.516	7.121	16.106		27.06	A
	ATOM	536	N	LEU			50.655	8.235	14.360		24.77	A
	ATOM	537	CA	LEU	Α	137	49.294	8.162	14.870	1.00	24.70	A
	ATOM	538	СВ	LEU			48.483	9.363	14.371		24.52	А
55												
55	ATOM	539	CG	LEU			49.050	10.760	14.662		26.67	A
	ATOM	540	CD1	LEU	Α	137	48.075	11.813	14.141	1.00	27.25	A
	ATOM	541	CD2	LEU	Α	137	49.279	10.945	16.155	1.00	27.09	A
	ATOM	542	C	LEU			48.592	6.868	14.473		25.20	A
	ATOM	543	0	LEU	А	T3/	48.619	6.469	13.309	T.00	25.99	A

	ATOM	544	N	ASP	Α	138	47.971	6.218	15.451	1.00 2	21.89	А
	ATOM	545	CA	ASP	Α	138	47.239	4.977	15.219	1.00 2		А
	ATOM	546	СВ	ASP	A	138	48.124	3.761	15.523	1.00 2	22.14	A
	ATOM	547	CG	ASP	Α	138	47.432	2.448	15.201	1.00 2	24.90	A
5	MOTA	548	OD1	ASP	Α	138	46.631	2.423	14.241	1.00 2	24.78	A
	ATOM	549	OD2	ASP	Α	138	47.691	1.443	15.897	1.00 2	25.39	A
	ATOM	550	С	ASP	Α	138	46.031	4.991	16.138	1.00 2	20.47	A
	ATOM	551	0	ASP	Α	138	45.967	4.248	17.118	1.00 1	L9.06	A
	MOTA	552	N	HIS	Α	139	45.075	5.852	15.810	1.00 1	L8.27	A
10	MOTA	553	CA	HIS	Α	139	43.869	6.016	16.606	1.00 1	18.21	A
	MOTA	554	СВ	HIS	Α	139	44.096	7.157	17.612	1.00 1	L5.84	A
	ATOM	555	CG	HIS	Α	139	42.985	7.332	18.600	1.00 1	L5.24	A
	ATOM	556	CD2	HIS	Α	139	42.884	6.964	19.900	1.00 1	L3.97	A
	MOTA	557		HIS			41.791	7.943	18.280	1.00 1		A
15	MOTA	558		HIS			41.002	7.944	19.341	1.00 1		A
	ATOM	559	NE2	HIS			41.641	7.356	20.336	1.00 1		A
	ATOM	560	С	HIS	Α	139	42.715	6.330	15.654	1.00 1		А
	ATOM	561	0			139	42.879	7.080	14.693	1.00 2		A
	ATOM	562	N			140	41.527	5.767	15.913	1.00 1		A
20	ATOM	563	CD			140	41.143	4.984	17.100	1.00 1		A
	ATOM	564	CA			140	40.367	6.001	15.048	1.00 1		A
	ATOM	565	СВ			140	39.273	5.157	15.704	1.00 1		A
	ATOM	566	CG			140	39.643	5.204	17.152	1.00 1		A
25	ATOM	567	C			140	39.914	7.441	14.803	1.00 1		A
25	ATOM	568	0			140	39.207	7.695	13.831	1.00 1		A
	ATOM	569	N			141	40.301	8.381	15.664	1.00 1		A
	ATOM	570	CA			141	39.874	9.767	15.477	1.00 1		A
	ATOM	571	CB			141	39.568	10.422	16.836	1.00 1		A
20	ATOM	572	CG			141	38.386	9.817	17.556	1.00 1		A
30	ATOM ATOM	573 574		PHE PHE			37.335 38.297	9.234 9.880	16.842 18.942	1.00 1 1.00 1		A A
	ATOM	575		PHE			36.215	8.727	17.502	1.00 1		A
	ATOM	576		PHE			37.178	9.375	19.615	1.00 1		A
	ATOM	577	CZ			141	36.135	8.799	18.893	1.00 1		A
35	ATOM	578	C			141	40.857	10.641	14.694	1.00 1		A
33	ATOM	579	0			141	40.799	11.871	14.761	1.00 1		A
	ATOM	580	N			142	41.748	10.011	13.941	1.00 1		A
	ATOM	581	CA			142	42.727	10.756	13.154	1.00 1		A
	ATOM	582	СВ			142	44.115	10.645	13.793	1.00 1		A
40	ATOM	583	CG			142	44.240	11.371	15.103	1.00 1		A
	ATOM	584		PHE			44.559	12.726	15.135	1.00 1		А
	ATOM	585	CD2				43.997	10.711	16.304	1.00 1		А
	ATOM	586	CE1	PHE	Α	142	44.632	13.417	16.347	1.00 1	L5.77	А
	ATOM	587	CE2	PHE	Α	142	44.065	11.393	17.522	1.00 1		А
45	ATOM	588	CZ			142	44.383	12.747	17.542	1.00 1		А
	ATOM	589	С	PHE	Α	142	42.793	10.231	11.729	1.00 1	19.12	A
	ATOM	590	0	PHE	Α	142	42.659	9.030	11.504	1.00 2	20.01	A
	MOTA	591	N	VAL	Α	143	42.978	11.135	10.769	1.00 1	L8.72	A
	MOTA	592	CA	VAL	Α	143	43.102	10.735	9.371	1.00 1	L8.52	A
50	ATOM	593	СВ	VAL	Α	143	43.294	11.961	8.440	1.00 2	20.66	A
	ATOM	594		VAL			43.843	11.521	7.080	1.00 2		A
	MOTA	595	CG2	VAL			41.958	12.673	8.252	1.00 2	22.97	A
	MOTA	596	С	VAL	Α	143	44.342	9.865	9.330	1.00 1	L8.68	A
_	MOTA	597	0			143	45.355	10.199	9.943	1.00 1		A
55	MOTA	598	N			144	44.259	8.745	8.623	1.00 1		A
	ATOM	599	CA	LYS			45.384	7.824	8.535	1.00 1		А
	ATOM	600	СВ			144	44.889	6.373	8.608	1.00 2		A
	ATOM	601	CG			144	46.017	5.340	8.557	1.00 2		A
	ATOM	602	CD	LYS	Α	144	45.491	3.912	8.674	1.00 3	34.16	А

	ATOM	603	CE	LYS I	A 144	46.631	2.896	8.577	1.00 37.67	A
	ATOM	604	ΝZ		A 144	46.138	1.484	8.629	1.00 39.02	A
	ATOM	605	С	LYS I	A 144	46.192	8.002	7.261	1.00 18.53	A
	ATOM	606	0	LYS	A 144	45.643	8.314	6.200	1.00 18.18	A
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5	MOTA	607	N		A 145	47.502	7.816	7.385	1.00 16.79	A
	ATOM	608	CA	LEU I	A 145	48.411	7.900	6.251	1.00 17.45	A
	ATOM	609	СВ	LEU	145	49.686	8.653	6.641	0.50 18.82	AC1
	ATOM	610	CG	LEU	145	50.734	8.902	5.549	0.50 20.23	AC1
	ATOM	611	CD1	LEU	145	51.836	9.799	6.093	0.50 18.83	AC1
10		612			145	51.317		5.069		
10	ATOM		CD2				7.581		0.50 19.79	AC1
	ATOM	613	С	LEU 2	A 145	48.739	6.450	5.907	1.00 19.19	A
	ATOM	614	0	LEH	A 145	49.451	5.772	6.659	1.00 17.36	A
	ATOM	615	N		A 146	48.215	5.972	4.782	1.00 17.28	A
	ATOM	616	CA	TYR 2	A 146	48.444	4.593	4.358	1.00 17.57	A
15	ATOM	617	СВ		A 146	47.288	4.098	3.486	1.00 17.74	A
13										
	ATOM	618	CG	TYR .	A 146	45.981	3.926	4.214	1.00 17.50	A
	ATOM	619	CD1	TYR I	A 146	45.099	4.995	4.377	1.00 16.50	A
	ATOM	620	CE1		A 146	43.881	4.827	5.039	1.00 17.10	А
	ATOM	621	CD2	TYR 2	A 146	45.620	2.686	4.735	1.00 18.28	A
20	ATOM	622	CE2	TYR :	A 146	44.411	2.506	5.399	1.00 19.84	A
_0										
	ATOM	623	CZ		A 146	43.547	3.576	5.544	1.00 17.53	A
	ATOM	624	OH	TYR 2	A 146	42.342	3.376	6.169	1.00 20.67	A
	ATOM	625	С	TVR	A 146	49.735	4.376	3.582	1.00 18.72	A
	ATOM	626	0	TYR .	A 146	50.382	3.338	3.715	1.00 19.51	A
25	ATOM	627	N	PHE 2	A 147	50.110	5.350	2.765	1.00 18.09	A
	ATOM	628	CA		A 147	51.307	5.203	1.952	1.00 17.20	А
	ATOM	629	СВ	PHE 2	A 147	51.007	4.258	0.783	1.00 16.77	A
	ATOM	630	CG	PHE	A 147	49.835	4.699	-0.070	1.00 17.75	A
	ATOM	631	CD1		A 147	49.967	5.752	-0.975	1.00 16.58	A
30	ATOM	632	CD2	PHE 2	A 147	48.595	4.075	0.053	1.00 18.07	A
	ATOM	633	CE1	PHE 2	147	48.886	6.178	-1.742	1.00 19.62	A
	ATOM	634	CE2	PHE I	A 147	47.503	4.492	-0.710	1.00 18.56	A
	ATOM	635	CZ	PHE 2	A 147	47.647	5.546	-1.610	1.00 19.27	A
	ATOM	636	С		A 147	51.768	6.533	1.395	1.00 17.13	A
35	ATOM	637	0	PHE 2	A 147	51.045	7.528	1.452	1.00 14.43	A
	ATOM	638	N	THR 2	A 148	52.981	6.534	0.854	1.00 17.12	A
		639			A 148	53.541	7.718	0.232	1.00 17.96	
	ATOM		CA							A
	ATOM	640	СВ	THR .	A 148	54.449	8.531	1.197	1.00 21.51	A
	ATOM	641	OG1	THR	A 148	55.605	7.760	1.537	1.00 18.83	A
40										
40	ATOM	642	CG2		A 148	53.700	8.897	2.472	1.00 19.60	A
	ATOM	643	С	THR I	A 148	54.386	7.262	-0.946	1.00 20.31	A
	ATOM	644	0	THR	A 148	54.860	6.124	-0.991	1.00 18.94	A
	ATOM	645	N		A 149	54.543	8.149	-1.916	1.00 19.16	A
	MOTA	646	CA	PHE 2	A 149	55.368	7.877	-3.073	1.00 18.01	A
45	ATOM	647	СВ	PHE	A 149	54.748	6.801	-3.989	1.00 17.23	А
15										
	ATOM	648	CG	PHE A	A 149	53.389	7.144	-4.544	1.00 16.88	A
	ATOM	649	CD1	PHE 2	A 149	53.262	7.888	-5.712	1.00 18.58	A
	ATOM	650		PHE 2		52.235	6.668	-3.927	1.00 17.31	А
	ATOM	651	CEI	PHE 2	A 149	52.007	8.149	-6.267	1.00 19.26	A
50	ATOM	652	CE2	PHE 2	A 149	50.972	6.923	-4.470	1.00 19.17	A
	ATOM	653	CZ		A 149	50.858	7.663	-5.642	1.00 19.60	A
	ATOM	654	С	PHE 2	A 149	55.542	9.205	-3.774	1.00 20.85	A
	ATOM	655	0		A 149	54.934	10.200	-3.376	1.00 19.76	A
	ATOM	656	N		A 150	56.398	9.241	-4.782	1.00 19.79	A
55	ATOM	657	CA	GLN Z	A 150	56.636	10.481	-5.497	1.00 24.03	A
	ATOM	658	СВ		A 150	57.659	11.347	-4.739	1.00 24.45	A
	ATOM	659	CG		A 150	58.986	10.645	-4.414	1.00 26.28	A
	ATOM	660	CD	GLN 3	A 150	59.988	11.558	-3.692	1.00 29.02	A
	ATOM	661		GLN .		60.693	12.353	-4.321	1.00 27.05	A
	AION	OOT	0111	י אודרט	1 100	50.095	12.555	4.JZI	1.00 21.00	Λ

	MOTA	662	NE2	GLN	A	150	60.042	11.449	-2.365		26.47	А
	MOTA	663	С			150	57.160	10.203	-6.885	1.00	23.88	A
	MOTA	664	0	GLN	Α	150	57.673	9.118	-7.158		24.79	A
	MOTA	665	N	ASP	Α	151	56.987	11.171	-7.774		25.88	A
5	MOTA	666	CA	ASP	Α	151	57.527	11.047	-9.117		26.49	A
	MOTA	667	СВ	ASP	Α	151	56.437	11.126	-10.199	1.00	24.54	A
	MOTA	668	CG	ASP			55.544	12.336	-10.064	1.00	24.95	A
	ATOM	669	OD1	ASP	Α	151	56.005	13.379	-9.561	1.00	22.44	A
	ATOM	670	OD2	ASP	Α	151	54.369	12.242	-10.490	1.00	25.72	A
10	ATOM	671	С	ASP	А	151	58.515	12.203	-9.220	1.00	28.63	A
	ATOM	672	0	ASP	Α	151	58.890	12.780	-8.194	1.00	27.83	A
	ATOM	673	N	ASP	Α	152	58.934	12.560	-10.426	1.00	29.21	A
	ATOM	674	CA	ASP	Α	152	59.907	13.636	-10.562	1.00	31.88	A
	ATOM	675	СВ	ASP	А	152	60.325	13.792	-12.026	1.00	33.94	A
15	ATOM	676	CG	ASP	А	152	61.033	12.564	-12.557	1.00	38.88	A
	ATOM	677	OD1	ASP	А	152	61.817	11.959	-11.791	1.00	39.67	A
	ATOM	678	OD2	ASP	Α	152	60.817	12.211	-13.738	1.00	41.57	A
	MOTA	679	С	ASP	Α	152	59.487	14.994	-10.013	1.00	30.90	A
	ATOM	680	0	ASP	Α	152	60.316	15.735	-9.482	1.00	31.69	A
20	ATOM	681	N	GLU	Α	153	58.207	15.322	-10.107	1.00	29.44	A
	ATOM	682	CA	GLU	Α	153	57.767	16.632	-9.646	1.00	28.69	A
	ATOM	683	СВ	GLU	Α	153	56.984	17.327	-10.766	1.00	32.90	A
	ATOM	684	CG	GLU	А	153	57.451	16.987	-12.183	1.00	40.57	А
	ATOM	685	CD	GLU	Α	153	56.920	15.643	-12.675	1.00	45.78	A
25	ATOM	686	OE1	GLU	Α	153	55.682	15.482	-12.760	1.00	48.91	A
	ATOM	687	OE2	GLU	Α	153	57.736	14.747	-12.979	1.00	48.95	A
	ATOM	688	С	GLU	Α	153	56.929	16.683	-8.372	1.00	26.43	A
	ATOM	689	0	GLU	Α	153	56.947	17.688	-7.660	1.00	25.08	A
	ATOM	690	N	LYS	Α	154	56.205	15.610	-8.069		22.39	А
30	ATOM	691	CA	LYS	Α	154	55.318	15.631	-6.912	1.00	21.43	A
	ATOM	692	СВ	LYS	Α	154	53.861	15.628	-7.398	1.00	20.33	А
	ATOM	693	CG	LYS	А	154	53.505	16.716	-8.403		21.92	А
	ATOM	694	CD	LYS			52.211	16.375	-9.146		19.70	А
	ATOM	695	CE	LYS	Α	154	51.775	17.503	-10.077	1.00	20.04	А
35	ATOM	696	NZ	LYS	Α	154	50.631	17.094	-10.951	1.00	19.97	А
	ATOM	697	С	LYS			55.458	14.522	-5.881		20.43	А
	ATOM	698	0	LYS			55.949	13.426	-6.173		21.13	А
	ATOM	699	N	LEU			54.985	14.832	-4.676		19.69	A
	ATOM	700	CA	LEU			54.950	13.900	-3.553		19.10	A
40	ATOM	701	СВ	LEU			55.362	14.588	-2.252		19.65	A
	ATOM	702	CG	LEU			56.740	15.234	-2.129		21.20	A
	ATOM	703		LEU			56.848	15.918	-0.770		23.42	A
	ATOM	704		LEU			57.816	14.174	-2.277		23.08	A
	ATOM	705	C	LEU			53.478	13.507	-3.427		18.87	A
45	ATOM	706	0			155	52.600	14.348	-3.620		18.61	A
	ATOM	707	N	TYR			53.209	12.249	-3.091		15.02	A
	ATOM	708	CA	TYR			51.834	11.783	-2.934		16.29	A
	ATOM	709	СВ	TYR			51.470	10.769	-4.029		14.20	A
	ATOM	710	CG	TYR			51.603	11.273	-5.449		17.29	A
50	ATOM	711		TYR			52.857	11.429	-6.045		16.46	A
20	ATOM	712		TYR			52.978	11.884	-7.360		18.68	A
	ATOM	713		TYR			50.474	11.588	-6.202		16.43	A
	ATOM	714		TYR			50.583	12.048	-7.512		16.31	A
	ATOM	715	CZ	TYR			51.835	12.192	-8.083		18.17	A
55	ATOM	716	OH	TYR			51.941	12.651	-9.371		17.47	A
55	ATOM	717	C	TYR			51.657	11.108	-1.572		16.32	A
	ATOM	718	0	TYR			52.412	10.197	-1.235		16.27	A
	ATOM	719	N	PHE			50.678	11.568	-0.792		15.47	A
	ATOM	720	CA	PHE	А	101	50.385	10.966	0.508	T.00	16.66	A

	ATOM	721	CB	PHE	Α	157	50.324	12.014	1.629	1.00	16.91	A
			CG	PHE			51.631					
	ATOM	722						12.708	1.907		18.96	A
	MOTA	723	CD1	PHE	Α	157	52.821	12.261	1.340	1.00	20.31	A
	ATOM	724	CD2	PHE	Δ	157	51.664	13.829	2.732	1 00	21.12	A
-												
5	ATOM	725		PHE			54.025	12.926	1.585		22.08	A
	ATOM	726	CE2	PHE	Α	157	52.865	14.500	2.982	1.00	22.18	A
	ATOM	727	CZ	PHE	7\	157	54.045	14.045	2.405	1 00	21.27	А
	ATOM	728	С	PHE	А	15/	49.016	10.308	0.404	1.00	16.52	A
	ATOM	729	0	PHE	Α	157	48.029	10.979	0.110	1.00	17.32	A
10	ATOM	730	N	GLY			48.953	9.002	0.644		15.97	А
10												
	MOTA	731	CA	GLY	Α	158	47.684	8.299	0.572	1.00	16.13	A
	ATOM	732	С	GLY	А	158	47.000	8.383	1.920	1.00	14.94	A
		733		GLY			47.445	7.756			16.28	
	ATOM		0						2.879			A
	MOTA	734	N	LEU	Α	159	45.915	9.145	1.989	1.00	13.50	A
15	ATOM	735	CA	LEU	Α	159	45.191	9.340	3.241	1.00	15.20	А
10												
	ATOM	736	СВ	LEU			45.031	10.835	3.517		14.20	A
	ATOM	737	CG	LEU	Α	159	46.270	11.726	3.385	1.00	19.00	A
	ATOM	738	CD1	LEU	Δ	159	45.847	13.188	3.477	1 00	17.12	А
	ATOM	739	CDZ	LEU			47.275	11.390	4.471		14.71	A
20	ATOM	740	С	LEU	Α	159	43.809	8.716	3.232	1.00	15.53	A
	ATOM	741	0	LEU	Δ	159	43.232	8.472	2.177	1 00	16.05	А
	ATOM	742	N	SER	А	160	43.268	8.469	4.418		15.86	A
	ATOM	743	CA	SER	Α	160	41.932	7.917	4.498	1.00	19.01	A
	ATOM	744	СВ	SER			41.566	7.582	5.949		22.90	А
25	ATOM	745	OG	SER	Α	160	41.901	8.629	6.833	1.00	24.18	A
	ATOM	746	С	SER	Α	160	40.987	8.968	3.924	1.00	20.43	A
		747		SER			41.213	10.173	4.062		19.96	
	ATOM		0									A
	ATOM	748	N	TYR	Α	161	39.945	8.508	3.250	1.00	19.20	A
	ATOM	749	CA	TYR	Δ	161	38.975	9.406	2.644	1.00	20.37	А
20												
30	ATOM	750	СВ	TYR			38.471	8.785	1.332		20.00	A
	MOTA	751	CG	TYR	Α	161	37.314	9.502	0.666	1.00	20.72	A
	ATOM	752	CD1	TYR	Δ	161	37.222	10.895	0.682	1 00	18.22	А
	ATOM	753	CEI	TYR	А	101	36.180	11.557	0.029		22.24	A
	ATOM	754	CD2	TYR	Α	161	36.333	8.784	-0.020	1.00	20.53	A
35	ATOM	755	CE2	TYR	Δ	161	35.287	9.436	-0.678		24.24	А
55												
	ATOM	756	CZ	TYR	А	101	35.218	10.822	-0.648	1.00	22.32	A
	ATOM	757	OH	TYR	Α	161	34.194	11.471	-1.298	1.00	23.03	A
	ATOM	758	С	TYR	7\	161	37.812	9.681	3.598	1 00	20.14	А
	ATOM	759	0	TYR			36.959	8.819	3.810		19.53	A
40	ATOM	760	N	ALA	Α	162	37.791	10.880	4.178	1.00	19.92	A
	ATOM	761	CA	ALA	Ζ.	162	36.721	11.271	5.099	1 00	21.07	А
	ATOM	762	СВ	ALA	А	162	37.187	12.419	6.002		19.60	A
	ATOM	763	С	ALA	Α	162	35.542	11.712	4.238	1.00	22.07	A
	ATOM	764	0	ALA			35.436	12.875	3.860		20.66	А
4.5												
45	ATOM	765	N	LYS	А	163	34.653	10.769	3.945	1.00	23.27	А
	ATOM	766	CA	LYS	Α	163	33.503	11.017	3.080	1.00	27.12	A
		767	СВ	LYS			32.663	9.741	2.963		29.68	
	ATOM											A
	ATOM	768	CG	LYS	Α	163	33.455	8.524	2.515	1.00	37.67	A
	ATOM	769	CD	LYS	A	163	32.556	7.310	2.321	1.00	42.24	A
50												
50	ATOM	770	CE	LYS			33.373	6.034	2.185		44.48	A
	ATOM	771	NZ	LYS	Α	163	34.143	5.735	3.430	1.00	44.88	A
	ATOM	772	С	LYS	А	163	32.581	12.186	3.411	1.00	25.78	А
	ATOM	773	0	LYS			32.103	12.863	2.506		26.53	A
	ATOM	774	N	ASN	Α	164	32.327	12.441	4.689	1.00	24.57	A
55	ATOM	775	CA	ASN			31.420	13.522	5.033	1.00	23.77	А
	ATOM	776	СВ	ASN			30.610	13.129	6.265		25.02	А
	ATOM	777	CG	ASN	Α	164	29.537	12.101	5.932	1.00	27.54	A
	ATOM	778	OD1	ASN			28.772	12.281	4.983	1.00	28.79	A
	ATOM	779	ИПΖ	ASN	А	T 0 4	29.475	11.024	6.704	T.00	27.13	A

	ATOM	780	С	ASN A	164	31.999	14.931	5.169	1.00 24.43	A
	ATOM	781	0	ASN A	164	31.306	15.856	5.589	1.00 23.98	A
	MOTA	782	N	GLY A		33.262	15.097	4.795	1.00 21.56	A
	ATOM	783	CA	GLY A	165	33.873	16.414	4.836	1.00 24.39	A
5	ATOM	784	С	GLY A	165	34.191	17.043	6.181	1.00 23.62	A
_	ATOM	785	0	GLY A		34.380	16.352	7.177	1.00 23.26	A
	ATOM	786	N	GLU A		34.234	18.373	6.186	1.00 23.22	A
	ATOM	787	CA	GLU A	166	34.563	19.176	7.362	1.00 24.54	A
	ATOM	788	СВ	GLU A	166	35.055	20.558	6.913	1.00 25.04	А
10	ATOM	789	CG	GLU A		36.419	20.569	6.229	1.00 26.48	
10										A
	ATOM	790	CD	GLU A	166	36.699	21.889	5.517	1.00 30.02	A
	MOTA	791	OE1	GLU A	166	36.081	22.906	5.889	1.00 29.33	A
	ATOM	792	OE 2	GLU A	166	37.544	21.916	4.596	1.00 30.48	A
	ATOM	793	С	GLU A		33.436	19.372	8.369	1.00 24.44	A
15	ATOM	794	0	GLU A	166	32.279	19.541	8.001	1.00 22.76	A
	ATOM	795	N	LEU A	167	33.791	19.370	9.649	1.00 22.95	A
	ATOM	796	CA	LEU A		32.813	19.581	10.707	1.00 22.26	А
	ATOM	797	СВ	LEU A		33.497	19.481	12.073	1.00 22.32	A
	MOTA	798	CG	LEU A	167	32.706	19.923	13.306	1.00 22.04	A
20	ATOM	799	CD1	LEU A	167	31.454	19.074	13.463	1.00 19.66	A
	ATOM	800	CD2	LEU A	167	33.597	19.805	14.537	1.00 21.17	A
	ATOM	801	С	LEU A		32.193	20.971	10.529	1.00 23.49	A
	ATOM	802	0	LEU A	167	31.047	21.209	10.907	1.00 23.56	A
	ATOM	803	N	LEU A	168	32.960	21.887	9.948	1.00 24.25	A
25	ATOM	804	CA	LEU A		32.473	23.245	9.722	1.00 26.64	A
23										
	MOTA	805	СВ	LEU A		33.560	24.099	9.066	1.00 25.62	A
	MOTA	806	CG	LEU A	168	33.198	25.546	8.707	1.00 27.34	A
	ATOM	807	CD1	LEU A	168	32.718	26.296	9.946	1.00 26.42	A
	ATOM	808		LEU A		34.418	26.238	8.119	1.00 26.74	A
20										
30	MOTA	809	С	LEU A		31.234	23.218	8.829	1.00 27.13	A
	ATOM	810	0	LEU A	168	30.297	23.989	9.030	1.00 26.01	A
	ATOM	811	N	LYS A	169	31.233	22.320	7.848	1.00 26.41	A
	ATOM	812	CA	LYS A		30.106	22.210	6.934	1.00 27.70	A
	MOTA	813	СВ	LYS A	169	30.324	21.064	5.945	1.00 30.49	A
35	ATOM	814	CG	LYS A	169	29.151	20.854	4.993	1.00 32.47	A
	ATOM	815	CD	LYS A	169	29.407	19.728	3.998	1.00 35.98	A
	ATOM	816	CE	LYS A		29.462	18.372	4.683	1.00 38.53	A
	MOTA	817	NZ	LYS A		29.622	17.263	3.702	1.00 41.00	A
	MOTA	818	С	LYS A	169	28.801	21.985	7.682	1.00 28.12	A
40	ATOM	819	0	LYS A	169	27.785	22.608	7.371	1.00 28.08	A
	ATOM	820	N	TYR A		28.826	21.094	8.668	1.00 26.53	A
	ATOM	821	CA	TYR A		27.624	20.791	9.434	1.00 26.95	A
	MOTA	822	CB	TYR A	170	27.810	19.476	10.193	1.00 25.03	A
	ATOM	823	CG	TYR A	170	27.898	18.300	9.251	1.00 26.65	A
45	ATOM	824		TYR A		26.745	17.661	8.790	1.00 28.27	А
73										
	ATOM	825		TYR A		26.814	16.642	7.839	1.00 26.85	A
	ATOM	826	CD2	TYR A	170	29.127	17.884	8.742	1.00 27.83	A
	ATOM	827	CE2	TYR A	170	29.209	16.869	7.792	1.00 27.19	A
	ATOM	828	CZ	TYR A		28.049	16.254	7.343	1.00 30.02	A
50										
50	ATOM	829	OH	TYR A	170	28.130	15.268	6.382	1.00 29.23	A
	ATOM	830	С	TYR A	170	27.229	21.918	10.376	1.00 27.59	A
	ATOM	831	0	TYR A		26.045	22.122	10.642	1.00 29.25	А
				ILE A				10.882	1.00 28.16	
	ATOM	832	N			28.208	22.660			A
	ATOM	833	CA	ILE A	171	27.883	23.770	11.763	1.00 29.03	A
55	ATOM	834	СВ	ILE A	171	29.151	24.435	12.337	1.00 27.51	A
	ATOM	835		ILE A		28.773	25.705	13.084	1.00 27.97	А
	ATOM	836		ILE A		29.872	23.458	13.272	1.00 26.70	A
	ATOM	837	CD1	ILE P	171	31.163	23.996	13.856	1.00 24.07	A
	ATOM	838	С	ILE A	171	27.094	24.796	10.944	1.00 31.41	A

	ATOM	839	0	ILE	Α	171	26.088	25.335	11.407	1.00	31.69	А
	ATOM	840	N	ARG	Α	172	27.546	25.047	9.719	1.00	33.21	A
	ATOM	841	CA	ARG	Α	172	26.874	26.000	8.844		36.54	A
	ATOM	842	СВ	ARG	Α	172	27.734	26.314	7.616	1.00	37.73	A
5	ATOM	843	CG	ARG	Α	172	29.057	27.011	7.912	1.00	41.65	A
	ATOM	844	CD	ARG	Α	172	29.708	27.492	6.616	1.00	45.29	A
	ATOM	845	NE	ARG	Α	172	31.037	28.070	6.812	1.00	48.51	A
	ATOM	846	CZ	ARG	Α	172	31.314	29.059	7.658	1.00	51.53	A
	ATOM	847	NH1	ARG	Α	172	30.355	29.593	8.406	1.00	53.75	A
10	ATOM	848	NH2	ARG	Α	172	32.553	29.526	7.748	1.00	51.21	A
	ATOM	849	С	ARG	Α	172	25.528	25.459	8.378	1.00	37.67	A
	ATOM	850	0	ARG	Α	172	24.550	26.200	8.288	1.00	39.09	A
	ATOM	851	N	LYS	Α	173	25.481	24.163	8.092	1.00	38.44	A
	MOTA	852	CA	LYS	Α	173	24.259	23.528	7.619	1.00	39.25	А
15	MOTA	853	СВ	LYS	Α	173	24.523	22.061	7.272	1.00	41.89	A
	ATOM	854	CG	LYS	Α	173	23.279	21.298	6.830	1.00	45.52	A
	MOTA	855	CD	LYS	Α	173	23.557	19.808	6.653	1.00	49.60	A
	MOTA	856	CE	LYS	Α	173	24.477	19.530	5.469	1.00	52.63	A
	ATOM	857	NZ	LYS	Α	173	23.855	19.894	4.160		54.61	A
20	ATOM	858	С	LYS			23.089	23.608	8.595		39.30	A
	ATOM	859	0	LYS	Α	173	21.981	23.960	8.201	1.00	39.62	A
	ATOM	860	N	ILE			23.320	23.282	9.863		37.96	A
	ATOM	861	CA	ILE			22.229	23.314	10.833		37.36	A
	ATOM	862	СВ	ILE			22.159	21.998	11.652		37.44	A
25	ATOM	863		ILE			22.058	20.802	10.709		38.37	A
	ATOM	864	CG1				23.397	21.850	12.532		37.25	A
	ATOM	865	CD1	ILE			23.355	20.620	13.418	1.00	36.85	A
	ATOM	866	С	ILE			22.259	24.492	11.801		36.71	A
	ATOM	867	0	ILE			21.448	24.556	12.724		38.05	A
30	ATOM	868	N	GLY			23.185	25.423	11.592		35.48	A
	ATOM	869	CA	GLY			23.265	26.585	12.462		35.29	A
	ATOM	870	С	GLY			24.053	26.360	13.737		35.06	A
	ATOM	871	0	GLY			25.066	27.019	13.970		37.46	A
	ATOM	872	N	SER	Α	176	23.581	25.441	14.571		33.94	A
35	ATOM	873	CA			176	24.253	25.113	15.822		32.84	A
	ATOM	874	СВ	SER			23.938	26.155	16.901		33.54	A
	ATOM	875	OG			176	22.599	26.056	17.347		34.86	A
	ATOM	876	С	SER			23.796	23.731	16.276		32.34	A
	ATOM	877	0	SER			22.726	23.263	15.884		32.82	A
40	MOTA	878	N	PHE			24.609	23.085	17.103		29.39	A
	ATOM	879	CA	PHE			24.313	21.743	17.597		27.20	A
	ATOM	880	СВ	PHE			25.621	20.989	17.865		26.39	A
	ATOM	881	CG	PHE			26.372	20.585	16.622		26.18	A
4.5	ATOM	882		PHE			26.210	21.277	15.426		25.30	A
45	ATOM	883		PHE			27.266	19.516	16.662		26.05	A
	ATOM	884		PHE			26.923	20.912	14.290		26.59	A
	ATOM	885		PHE			27.986	19.143	15.532		26.06	A
	ATOM	886	CZ	PHE			27.815	19.841	14.343		25.42	A
5 0	ATOM	887	С	PHE			23.500	21.752	18.884		27.00	A
50	ATOM	888	0	PHE			23.704	22.610	19.747		26.48	A
	ATOM	889	N	ASP			22.578	20.802	19.022		26.70	A
	ATOM	890	CA	ASP			21.816	20.729	20.260		26.35	A
	ATOM	891	СВ	ASP			20.621	19.773	20.142		29.90	A
	ATOM	892	CG	ASP			21.020	18.372	19.720		32.28	A
55	ATOM	893		ASP			22.157	17.949	20.014		35.21	A
	ATOM	894		ASP			20.179	17.683	19.105		34.79	A
	ATOM	895	С	ASP			22.810	20.228	21.311		25.03	A
	ATOM	896	0	ASP			23.974	19.968	20.992		21.24	A
	ATOM	897	N	GLU	А	179	22.361	20.083	22.552	1.00	23.60	A

	MOTA	898	CA	GLU A	179	23.247	19.644	23.619		25.18	A
	ATOM	899	CB	GLU A	179	22.542	19.770	24.971	1.00	27.60	A
	ATOM	900	CG	GLU A	179	23.324	19.176	26.130	1.00	32.58	A
	ATOM	901	CD	GLU A		22.997	19.845	27.449		35.82	A
_											
5	MOTA	902	OE1	GLU A		21.825	20.224	27.645		35.95	A
	MOTA	903	OE2	GLU A	179	23.912	19.984	28.291	1.00	38.19	A
	ATOM	904	С	GLU A	179	23.808	18.235	23.450	1.00	24.08	A
	ATOM	905	0	GLU A	179	24.977	17.989	23.756	1.00	22.79	A
	ATOM	906	N	THR A		22.983	17.316	22.961		23.36	A
10											
10	MOTA	907	CA	THR A		23.412	15.935	22.761		22.15	A
	MOTA	908	СВ	THR A	180	22.224	15.054	22.320		23.77	A
	ATOM	909	og1	THR A	180	21.222	15.075	23.341	1.00	26.37	A
	ATOM	910	CG2	THR A	180	22.670	13.616	22.088	1.00	22.66	A
	ATOM	911	С	THR A	180	24.533	15.830	21.724		22.01	A
15	ATOM	912		THR A		25.533	15.141	21.944		19.87	
13			0								A
	MOTA	913	N	CYS A		24.365	16.511	20.596		21.21	A
	ATOM	914	CA	CYS A	181	25.372	16.480	19.541	1.00	22.22	A
	ATOM	915	СВ	CYS A	181	24.800	17.065	18.250	1.00	24.62	A
	ATOM	916	SG	CYS A	181	23.435	16.080	17.560	1.00	29.50	A
20	ATOM	917	C	CYS A		26.633	17.232	19.954		23.07	A
20											
	MOTA	918	0	CYS A		27.746	16.827	19.608		23.95	A
	ATOM	919	N	THR A		26.463	18.325	20.695		22.76	A
	ATOM	920	CA	THR A	182	27.606	19.103	21.161	1.00	21.49	A
	ATOM	921	СВ	THR A	182	27.167	20.346	21.978	1.00	21.37	A
25	ATOM	922	OG1	THR A		26.459	21.262	21.134		22.50	A
23	ATOM	923	CG2	THR A		28.379	21.046	22.565		18.36	A
	MOTA	924	С	THR A		28.454	18.215	22.071		21.48	A
	MOTA	925	0	THR A	182	29.669	18.090	21.894	1.00	19.95	A
	MOTA	926	N	ARG A	183	27.798	17.602	23.050	1.00	18.97	A
30	ATOM	927	CA	ARG A	183	28.468	16.723	23.996	1.00	19.39	A
-	ATOM	928	СВ	ARG	183	27.455	16.140	24.984		19.46	AC1
	ATOM	929	CG	ARG	183	28.030	15.062	25.887		18.77	AC1
	MOTA	930	CD	ARG	183	27.021	14.571	26.925		21.19	AC1
	ATOM	931	NE	ARG	183	26.605	15.642	27.824	0.50	19.46	AC1
35	ATOM	932	CZ	ARG	183	25.496	16.362	27.679	0.50	20.45	AC1
	ATOM	933	NH1	ARG	183	24.672	16.123	26.666	0.50	19.81	AC1
	ATOM	934		ARG	183	25.224	17.338	28.539		17.11	AC1
	ATOM	935	С	ARG A		29.206	15.577	23.302		20.02	A
	MOTA	936	0	ARG A		30.383	15.333	23.573		19.97	A
40	ATOM	937	N	PHE A	184	28.520	14.871	22.409	1.00	19.24	A
	ATOM	938	CA	PHE A	184	29.144	13.746	21.722	1.00	18.04	A
	MOTA	939	СВ	PHE A	184	28.158	13.078	20.764	1.00	21.05	A
	ATOM	940	CG	PHE A		28.719	11.857	20.098		22.67	A
								20.754			
4.5	ATOM	941		PHE A		28.717	10.630			22.97	A
45	MOTA	942		PHE A		29.317	11.949	18.850		19.97	A
	ATOM	943	CE1	PHE A	184	29.308	9.510	20.176	1.00	23.53	A
	ATOM	944	CE2	PHE A	184	29.915	10.833	18.263	1.00	24.11	A
	ATOM	945	CZ	PHE A		29.910	9.613	18.928		22.97	A
	ATOM	946	C	PHE A		30.403	14.127	20.941		17.99	A
50											
50	MOTA	947	0	PHE A		31.461	13.531	21.130		18.89	A
	MOTA	948	N	TYR A	185	30.292	15.110	20.056	1.00	15.73	A
	ATOM	949	CA	TYR A	185	31.443	15.519	19.265	1.00	15.72	A
	ATOM	950	СВ	TYR A	185	30.992	16.413	18.111	1.00	17.33	A
	ATOM	951	CG	TYR A		30.364	15.584	17.015		19.37	A
55											
55	ATOM	952		TYR A		31.159	14.809	16.168		16.53	A
	MOTA	953		TYR A		30.590	13.952	15.232		18.12	A
	MOTA	954	CD2	TYR A	185	28.976	15.484	16.892	1.00	18.18	A
	ATOM	955	CE2	TYR A	185	28.398	14.623	15.956	1.00	18.90	A
	ATOM	956	CZ	TYR A		29.211	13.861	15.133		18.41	А

	ATOM	957	ОН	TYR A	185	28.650	12.995	14.218	1.00 20.48	A
	ATOM	958	C	TYR A		32.544	16.172	20.083	1.00 15.79	A
	ATOM	959	0	TYR A		33.720	16.015	19.766	1.00 17.69	A
_	ATOM	960	N	THR A		32.176	16.887	21.142	1.00 15.68	A
5	ATOM	961	CA	THR A		33.184	17.504	21.997	1.00 16.03	A
	ATOM	962	СВ	THR A		32.559	18.403	23.094	1.00 16.62	A
	MOTA	963		THR A		31.866	19.503	22.481	1.00 14.79	A
	MOTA	964	CG2	THR A	186	33.656	18.953	24.019	1.00 14.68	A
	ATOM	965	С	THR A	186	33.954	16.375	22.680	1.00 15.59	A
10	ATOM	966	0	THR A	186	35.176	16.443	22.823	1.00 13.77	A
	ATOM	967	N	ALA A	187	33.234	15.333	23.097	1.00 14.06	A
	ATOM	968	CA	ALA A	187	33.869	14.196	23.757	1.00 14.74	А
	ATOM	969	СВ	ALA A	187	32.810	13.195	24.224	1.00 14.32	A
	ATOM	970	С	ALA A		34.875	13.509	22.821	1.00 14.41	A
15	ATOM	971	0	ALA A		35.972	13.136	23.247	1.00 15.61	A
13	ATOM	972	N	GLU A		34.516	13.340	21.549	1.00 14.01	A
		973		GLU A		35.443	12.704	20.615	1.00 14.01	A
	ATOM		CA							
	ATOM	974	СВ	GLU A		34.782	12.449	19.251	1.00 12.85	A
• •	ATOM	975	CG	GLU A		33.622	11.454	19.282	1.00 12.71	А
20	ATOM	976	CD	GLU A		33.464	10.685	17.979	1.00 15.01	A
	MOTA	977	OE1	GLU A		33.687	11.275	16.899	1.00 13.21	A
	ATOM	978	OE2	GLU A	188	33.110	9.484	18.031	1.00 17.69	A
	ATOM	979	С	GLU A	188	36.682	13.582	20.436	1.00 13.34	A
	ATOM	980	0	GLU A	188	37.803	13.085	20.408	1.00 14.69	A
25	ATOM	981	N	ILE A	189	36.486	14.893	20.326	1.00 13.52	A
	ATOM	982	CA	ILE A	189	37.627	15.787	20.159	1.00 13.35	A
	ATOM	983	СВ	ILE A		37.169	17.247	19.939	1.00 13.95	A
	ATOM	984	CG2			38.381	18.165	19.822	1.00 12.47	A
	ATOM	985		ILE A		36.302	17.332	18.671	1.00 13.44	A
30	ATOM	986		ILE A		35.588	18.664	18.491	1.00 13.44	A
30		987								
	ATOM		C	ILE A		38.530	15.702	21.394	1.00 14.63	A
	ATOM	988	0	ILE A		39.753	15.595	21.271	1.00 12.97	A
	ATOM	989	N	VAL A		37.927	15.751	22.582	1.00 14.35	A
	ATOM	990	CA	VAL A		38.684	15.655	23.832	1.00 13.22	A
35	MOTA	991	СВ	VAL A		37.743	15.690	25.061	1.00 14.28	A
	ATOM	992		VAL A		38.509	15.267	26.326	1.00 15.08	A
	ATOM	993	CG2	VAL A	190	37.160	17.082	25.233	1.00 12.08	A
	ATOM	994	С	VAL A	190	39.468	14.338	23.859	1.00 14.61	A
	ATOM	995	0	VAL A	190	40.634	14.304	24.250	1.00 13.72	A
40	ATOM	996	N	SER A		38.825	13.254	23.432	1.00 15.26	A
	ATOM	997	CA	SER A		39.478	11.943	23.421	1.00 16.81	A
	ATOM	998	СВ	SER	191	38.470	10.857	23.041	0.50 16.14	AC1
	ATOM	999	OG	SER	191	39.018	9.569	23.238	0.50 16.94	AC1
	ATOM	1000	C	SER A		40.649	11.928	22.441	1.00 16.58	
15										A
45	ATOM	1001	0	SER A		41.697	11.335	22.713	1.00 13.96	A
	ATOM	1002	N	ALA A		40.468	12.586	21.300	1.00 15.26	A
	MOTA	1003	CA	ALA A		41.518	12.645	20.292	1.00 14.37	A
	MOTA	1004	СВ	ALA A	192	40.989	13.296	19.016	1.00 14.43	A
	ATOM	1005	С	ALA A	192	42.695	13.440	20.845	1.00 16.46	A
50	ATOM	1006	0	ALA A	192	43.851	13.038	20.697	1.00 17.96	A
	ATOM	1007	N	LEU A	193	42.401	14.563	21.496	1.00 15.02	A
	ATOM	1008	CA	LEU A	193	43.459	15.392	22.067	1.00 15.42	A
	ATOM	1009	СВ	LEU A		42.884	16.712	22.600	1.00 12.88	A
	ATOM	1010	CG	LEU A		42.445	17.721	21.525	1.00 15.97	A
55	ATOM	1011		LEU A		41.869	18.979	22.190	1.00 13.97	A
55	ATOM	1012		LEU A		43.642	18.088	20.655	1.00 13.57	A
			CDZ							
	MOTA	1013		LEU A		44.211	14.659	23.174	1.00 14.49	A
	MOTA	1014	0	LEU A		45.427	14.813	23.310	1.00 16.56	A
	ATOM	1015	N	GLU A	194	43.500	13.870	23.975	1.00 13.96	А

	ATOM	1016	CA	GLU	Α	194	44.179	13.123	25.032	1.00	14.08	А
	ATOM	1017	СВ	GLU			43.190	12.295	25.857		14.65	A
	ATOM	1018	CG	GLU			43.882	11.301	26.789		17.09	A
	ATOM	1019	CD	GLU			42.924	10.592	27.730		19.59	A
5				GLU					27.730			
3	ATOM	1020					41.809	10.237			19.25	A
	ATOM	1021		GLU			43.302	10.380	28.906		20.20	A
	MOTA	1022	С	GLU			45.208	12.199	24.386		13.57	A
	MOTA	1023	0	GLU			46.337	12.093	24.847		14.23	A
	MOTA	1024	N	TYR			44.822	11.544	23.301		14.89	A
10	MOTA	1025	CA	TYR	Α	195	45.743	10.642	22.618		16.58	А
	ATOM	1026	СВ	TYR	Α	195	45.030	9.910	21.488	1.00	17.29	A
	ATOM	1027	CG	TYR	Α	195	45.956	9.058	20.649	1.00	17.92	A
	ATOM	1028	CD1	TYR	Α	195	46.347	7.788	21.077	1.00	17.96	A
	ATOM	1029	CE1	TYR	Α	195	47.203	6.996	20.304	1.00	19.77	А
15	ATOM	1030	CD2	TYR	Α	195	46.445	9.524	19.428		16.67	А
	ATOM	1031		TYR			47.299	8.744	18.650		18.51	А
	ATOM	1032	CZ	TYR			47.671	7.481	19.094		20.24	A
	ATOM	1033	OH	TYR			48.506	6.705	18.325		21.89	A
	ATOM	1033	C	TYR			46.917	11.419	22.035		16.98	A
20		1034	0	TYR				11.419	22.203		14.61	
20	ATOM						48.081					A
	ATOM	1036	N	LEU			46.599	12.507	21.347		16.30	A
	ATOM	1037	CA	LEU			47.619	13.328	20.720		18.15	A
	MOTA	1038	СВ	LEU			46.969	14.502	19.982		18.59	A
	MOTA	1039	CG	LEU			47.834	15.203	18.935		22.51	А
25	MOTA	1040		LEU			48.222	14.206	17.841		20.94	A
	MOTA	1041	CD2	LEU			47.060	16.375	18.338		22.98	A
	MOTA	1042	С	LEU	Α	196	48.592	13.844	21.763	1.00	17.75	A
	MOTA	1043	0	LEU	Α	196	49.801	13.644	21.649	1.00	18.33	A
	ATOM	1044	N	HIS	Α	197	48.064	14.495	22.792	1.00	17.12	A
30	ATOM	1045	CA	HIS	Α	197	48.913	15.042	23.842	1.00	18.47	A
	ATOM	1046	СВ	HIS	Α	197	48.069	15.866	24.817	1.00	15.90	A
	ATOM	1047	CG	HIS	Α	197	47.571	17.152	24.231	1.00	19.15	A
	ATOM	1048	CD2	HIS	Α	197	47.830	17.745	23.038	1.00	18.22	А
	ATOM	1049		HIS			46.704	17.992	24.897		17.47	А
35	ATOM	1050		HIS			46.450	19.047	24.139		19.74	А
	ATOM	1051		HIS			47.119	18.921	23.007		15.69	A
	ATOM	1052	C	HIS			49.696	13.958	24.572		19.40	A
	ATOM	1053	0	HIS			50.823	14.192	25.021		19.42	A
	ATOM	1053	N	GLY			49.106	12.770	24.679		18.59	A
40	ATOM	1055	CA	GLY			49.793	11.675	25.339		19.60	A
40		1056		GLY			51.075	11.307	24.612		21.86	
	ATOM	1056	C									A
	ATOM		0	GLY				10.682			23.09	A
	ATOM	1058	N	LYS			51.174	11.687	23.341		22.81	A
4.5	ATOM	1059	CA	LYS			52.368	11.401	22.549		24.43	A
45	MOTA	1060	СВ	LYS			51.990	10.905	21.154		26.00	А
	MOTA	1061	CG	LYS			51.378	9.520	21.133		30.98	A
	MOTA	1062	CD	LYS			51.291	9.002	19.708		36.85	A
	MOTA	1063	CE	LYS	Α	199	50.832	7.559	19.682	1.00	40.37	A
	MOTA	1064	NZ	LYS	Α	199	51.646	6.691	20.581	1.00	43.48	A
50	MOTA	1065	С	LYS	Α	199	53.253	12.631	22.414	1.00	23.88	A
	MOTA	1066	0	LYS	Α	199	54.144	12.669	21.568	1.00	24.97	A
	MOTA	1067	N	GLY	Α	200	52.997	13.638	23.243	1.00	24.00	А
	ATOM	1068	CA	GLY			53.790	14.853	23.203		22.12	А
	ATOM	1069	С	GLY			53.665	15.632	21.907		22.14	А
55	ATOM	1070	0	GLY			54.632	16.231	21.439		22.41	А
	ATOM	1071	N	ILE			52.475	15.630	21.320		20.00	A
	ATOM	1072	CA	ILE			52.252	16.355	20.080		18.93	A
	ATOM	1073	CB	ILE			51.784	15.414	18.955		19.70	A
	ATOM	1074		ILE			51.414	16.226	17.716		20.12	A
	111011	TO / T	JU2	للبد	41		~ .	10.220	I, • / I O		20.12	А

	ATOM	1075	CG1	ILE	Α	201	52.880	14.395	18.636	1.00	20.03	A
	ATOM	1076	CD1	ILE	7	201	52.408	13.258	17.745	1 00	22.75	Α
	ATOM	1077	С	ILE			51.193	17.425	20.270		19.87	Α
	ATOM	1078	0	ILE	Α	201	50.121	17.161	20.817	1.00	20.08	Α
5	ATOM	1079	N	ILE	Δ	202	51.508	18.633	19.815	1 00	19.94	Α
,							50.601					
	ATOM	1080	CA	ILE				19.772	19.891		20.45	А
	MOTA	1081	СВ	ILE	Α	202	51.352	21.040	20.356	1.00	22.21	Α
	ATOM	1082	CG2	ILE	Α	202	50.381	22.220	20.470	1.00	22.67	A
	ATOM	1083		ILE			52.033	20.775	21.700		24.19	A
1.0												
10	ATOM	1084	CDI	ILE	А	202	52.914	21.920	22.169	1.00	25.39	A
	ATOM	1085	С	ILE	Α	202	50.105	19.999	18.464	1.00	20.71	A
	ATOM	1086	0	ILE	Δ	202	50.910	20.067	17.538	1.00	19.48	Α
											18.65	
	ATOM	1087	N	HIS			48.795	20.108	18.270			A
	MOTA	1088	CA	HIS	Α	203	48.280	20.319	16.919	1.00	18.02	A
15	ATOM	1089	СВ	HIS	Α	203	46.775	20.057	16.874	1.00	16.31	Α
	ATOM	1090	CG	HIS	Δ	203	46.199	20.136	15.495	1 00	18.36	Α
	ATOM	1091		HIS			46.043	21.186	14.655		16.42	А
	MOTA	1092	ND1	HIS	Α	203	45.759	19.026	14.806	1.00	19.50	Α
	ATOM	1093	CE1	HIS	Α	203	45.359	19.389	13.600	1.00	17.64	Α
20	ATOM	1094		HIS			45.522	20.694	13.483		20.87	A
20												
	ATOM	1095	С	HIS	А	203	48.589	21.738	16.405		18.92	А
	MOTA	1096	0	HIS	Α	203	49.073	21.906	15.282	1.00	16.21	Α
	ATOM	1097	N	ARG	Δ	204	48.301	22.744	17.232	1.00	18.60	Α
		1098					48.552					
	ATOM		CA	ARG				24.157	16.914		19.81	A
25	MOTA	1099	СВ	ARG	Α	204	49.998	24.365	16.458	1.00	21.61	Α
	ATOM	1100	CG	ARG	Α	204	51.024	24.137	17.550	1.00	23.82	A
	ATOM	1101	CD	ARG	Δ	204	52.323	24.870	17.252	1 00	27.62	Α
	ATOM	1102	NE	ARG			52.932	24.449	15.994		29.43	А
	MOTA	1103	CZ	ARG	Α	204	54.125	24.861	15.572	1.00	33.10	Α
30	ATOM	1104	NH1	ARG	Α	204	54.835	25.706	16.311	1.00	32.12	Α
	ATOM	1105		ARG			54.614	24.426	14.418		30.25	A
	ATOM	1106	С	ARG			47.624	24.830	15.905		20.03	А
	ATOM	1107	0	ARG	Α	204	47.711	26.038	15.698	1.00	20.88	Α
	ATOM	1108	N	ASP	Α	205	46.755	24.071	15.255	1.00	18.96	A
35	ATOM	1109		ASP			45.828	24.692	14.325		17.90	A
33			CA									
	ATOM	1110	СВ	ASP	Α	205	46.418	24.741	12.914	1.00	18.95	Α
	ATOM	1111	CG	ASP	Α	205	45.655	25.688	12.008	1.00	20.36	A
	ATOM	1112	OD1	ASP	Δ	205	44.939	26.560	12.545	1.00	20.35	A
		1113		ASP			45.772	25.573	10.771		22.49	A
40	ATOM											
40	ATOM	1114	С	ASP			44.500	23.956	14.328	1.00	19.60	Α
	ATOM	1115	0	ASP	Α	205	43.876	23.751	13.287	1.00	21.53	A
	ATOM	1116	N	LEU	Δ	206	44.063	23.569	15.521	1.00	18.53	Α
				LEU								
	ATOM	1117	CA				42.813	22.851	15.667		19.18	A
	ATOM	1118	СВ	LEU			42.693	22.295	17.087		18.94	А
45	ATOM	1119	CG	LEU	Α	206	41.511	21.358	17.346	1.00	23.10	A
	ATOM	1120	CD1	LEU			41.615	20.142	16.436		23.01	Α
	ATOM	1121		LEU			41.504	20.933	18.808		22.97	А
	MOTA	1122	С	LEU	Α	206	41.639	23.772	15.361	1.00	19.05	A
	MOTA	1123	0	LEU	Α	206	41.556	24.880	15.886	1.00	19.25	Α
50	ATOM	1124	N	LYS			40.740	23.307	14.500		17.54	A
50												
	ATOM	1125	CA	LYS			39.564	24.081	14.110		18.60	А
	MOTA	1126	СВ	LYS	Α	207	39.980	25.248	13.196	1.00	18.98	Α
	ATOM	1127	CG	LYS	Α	207	40.786	24.817	11.982	1.00	18.20	Α
	ATOM	1128	CD	LYS			41.246	26.000	11.139		21.42	A
55	ATOM	1129	CE	LYS			42.223	25.537	10.062		23.21	А
	ATOM	1130	NZ	LYS	Α	207	42.561	26.604	9.084	1.00	29.61	Α
	ATOM	1131	С	LYS	Α	207	38.566	23.181	13.388		18.18	А
	ATOM	1132	0	LYS			38.921	22.100	12.915		18.11	A
	ATOM	1133	N	PRO	А	∠∪४	37.298	23.614	13.293	T.00	20.26	А

	ATOM	1134	CD	PRO A	208	36.7	13 24.8	33 13.88	2 1.00	18.79	A
	ATOM	1135	CA	PRO A		36.2				19.67	А
	ATOM	1136	CB	PRO A		35.0				19.45	A
~	ATOM	1137	CG	PRO A		35.2				21.81	A -
5	ATOM	1138	С	PRO A		36.6				21.04	A
	ATOM	1139	0	PRO A		36.2				21.19	A
	MOTA	1140	N	GLU A	209	37.4	74 23.1	88 10.52	3 1.00	21.69	A
	ATOM	1141	CA	GLU A	209	37.9	28 22.8	72 9.17	1.00	22.64	A
	ATOM	1142	СВ	GLU	209	38.6	44 24.0	84 8.55	0.50	23.65	AC1
10	ATOM	1143	CG	GLU	209	39.2				27.24	AC1
	ATOM	1144	CD	GLU	209	40.1				29.40	AC1
	ATOM	1145		GLU	209	39.6				29.68	AC1
		1146		GLU	209					30.07	
	ATOM					41.3					AC1
1.5	ATOM	1147	С	GLU A		38.8				22.28	A
15	ATOM	1148	0	GLU A		38.9				21.36	А
	ATOM	1149	N	ASN A	210	39.6		90 10.26	3 1.00	19.90	A
	MOTA	1150	CA	ASN A	210	40.5	74 20.4	12 10.43	6 1.00	19.44	A
	ATOM	1151	СВ	ASN A	210	41.7	44 20.9	12 11.28	7 1.00	20.07	A
	ATOM	1152	CG	ASN A	210	42.7	46 21.6	98 10.47	9 1.00	25.77	A
20	ATOM	1153	OD1	ASN A		43.5				26.73	А
	ATOM	1154		ASN A		42.6				25.15	A
	ATOM	1155	C	ASN A		40.0				18.63	A
	ATOM	1156	0	ASN A		40.7				18.29	A
	ATOM	1157	N	ILE A		38.7				16.31	A
25	ATOM	1158	CA	ILE A		38.0				15.49	A
	ATOM	1159	СВ	ILE A		37.3			4 1.00	15.40	A
	MOTA	1160	CG2	ILE A	211	36.5	82 17.3	11 13.95	1.00	14.59	A
	ATOM	1161	CG1	ILE A	211	38.3	42 19.0	46 14.36	5 1.00	15.91	A
	ATOM	1162	CD1	ILE A	211	37.7	20 19.6	69 15.59	1.00	15.98	А
30	ATOM	1163	С	ILE A		37.1				17.26	A
	ATOM	1164	0	ILE A		35.9				18.16	A
	ATOM	1165	N	LEU A		37.5				15.97	A
	ATOM	1166	CA	LEU A		36.7				17.08	A
	ATOM	1167	СВ	LEU A		37.6				17.78	A
35	ATOM	1168	CG	LEU A		38.7				18.92	A
	ATOM	1169		LEU A		39.4				22.09	A
	MOTA	1170	CD2	LEU A	212	38.1	88 17.4	82 7.16	6 1.00	19.91	A
	ATOM	1171	С	LEU A	212	35.8	43 14.8	25 9.83	7 1.00	18.35	A
	MOTA	1172	0	LEU A	212	35.9	57 14.4	33 11.00	2 1.00	19.39	A
40	ATOM	1173	N	LEU A		34.9	15 14.3	68 9.00	0 1.00	17.84	А
	ATOM	1174	CA	LEU A	213	33.9				19.94	A
	ATOM	1175	СВ	LEU A		32.5				20.84	A
	ATOM	1176	CG	LEU A		32.3				20.31	A
	ATOM	1177		LEU A		31.1				22.75	A
15											
45	ATOM	1178		LEU A		32.3				23.93	A
	ATOM	1179	С	LEU A		33.9				20.98	A
	ATOM	1180	0	LEU A	. 213	33.7				19.55	A
	MOTA	1181	N	ASN A	214	34.0	88 10.9	70 8.93	5 1.00	20.44	A
	ATOM	1182	CA	ASN A	214	34.0	55 9.8	14 8.04	9 1.00	23.77	A
50	ATOM	1183	СВ	ASN A	214	34.7	45 8.5	96 8.67	4 1.00	25.30	A
	ATOM	1184	CG	ASN A		34.0				32.04	А
	ATOM	1185		ASN A		32.9				34.43	A
	ATOM	1186		ASN A		34.8				33.85	A
<i></i>	ATOM	1187	C	ASN A		32.6				24.07	A
55	ATOM	1188	0	ASN A		31.6				19.94	A
	ATOM	1189	N	GLU A		32.4				25.77	A
	ATOM	1190	CA	GLU A	215	31.1				28.69	А
	ATOM	1191	СВ	GLU A	215	31.2	75 6.7	96 5.51	3 1.00	31.98	A
	ATOM	1192	CG	GLU A	215	29.9	70 6.3	34 4.89	6 1.00	40.22	A

	ATOM	1193	CD	GT.II	Δ	215	30.182	5.312	3.795	1.00	44 27	А
	ATOM	1194		GLU			30.817	4.268	4.065	1.00		A
	ATOM	1195		GLU			29.716	5.556	2.660	1.00		A
	ATOM	1196	C			215	30.188	7.673	7.601	1.00		A
5												
3	ATOM	1197	0			215	28.971	7.769	7.447	1.00		A
	ATOM	1198	N			216	30.737	7.287	8.752	1.00		A
	ATOM	1199	CA	ASP			29.914	6.953	9.917	1.00		A
	ATOM	1200	СВ	ASP			30.538	5.795	10.696	1.00		A
10	ATOM	1201	CG			216	30.390	4.466	9.979	1.00		А
10	ATOM	1202		ASP			29.274	4.170	9.499	1.00		A
	ATOM	1203		ASP			31.382	3.710	9.902	1.00		A
	ATOM	1204	С			216	29.697	8.135	10.862	1.00		А
	ATOM	1205	0	ASP			29.136	7.984	11.950	1.00		A
	ATOM	1206	N	MET	Α	217	30.156	9.306	10.441	1.00	23.02	A
15	ATOM	1207	CA	MET	Α	217	30.015	10.527	11.218	1.00	21.83	A
	ATOM	1208	СВ	MET	Α	217	28.537	10.789	11.517	1.00	23.24	A
	ATOM	1209	CG	MET	Α	217	27.742	11.186	10.274	1.00	22.98	A
	ATOM	1210	SD	MET	Α	217	28.464	12.616	9.430	1.00	27.57	А
	ATOM	1211	CE	MET	Α	217	27.679	13.974	10.332	1.00	26.68	А
20	ATOM	1212	С	MET	Α	217	30.844	10.618	12.502	1.00	21.51	А
	ATOM	1213	0	MET			30.474	11.323	13.440	1.00	18.62	А
	ATOM	1214	N	HIS			31.957	9.892	12.544	1.00		A
	ATOM	1215	CA	HIS			32.873	9.964	13.678	1.00		A
	ATOM	1216	CB	HIS			33.482	8.594	13.977	1.00		A
25	ATOM	1217	CG	HIS			32.551	7.667	14.698	1.00		A
23	ATOM	1218		HIS			31.910	6.547	14.287	1.00		A
	ATOM	1219		HIS			32.177	7.863	16.011	1.00		A
										1.00		
	ATOM	1220		HIS			31.348	6.902	16.379			A
20	ATOM	1221		HIS			31.168	6.091	15.351	1.00		A
30	ATOM	1222	C	HIS			33.947	10.921	13.172	1.00		A
	ATOM	1223	0	HIS			34.170	11.004	11.965	1.00		A
	ATOM	1224	N			219	34.617	11.638	14.067	1.00		A
	ATOM	1225	CA			219	35.628	12.586	13.618	1.00		A
	ATOM	1226	СВ			219	35.987	13.614	14.716	1.00		A
35	ATOM	1227	CG2				34.722	14.305	15.221	1.00		A
	ATOM	1228	CG1	ILE			36.734	12.919	15.864	1.00		A
	ATOM	1229	CD1				37.279	13.885	16.911	1.00		A
	MOTA	1230	С			219	36.929	11.944	13.161	1.00		A
	ATOM	1231	0			219	37.238	10.799	13.500	1.00	15.88	A
40	ATOM	1232	N	GLN	Α	220	37.677	12.711	12.378	1.00	15.62	A
	ATOM	1233	CA	GLN	Α	220	38.980	12.316	11.876	1.00	17.84	A
	ATOM	1234	СВ	GLN	Α	220	38.872	11.595	10.525	1.00	20.00	A
	ATOM	1235	CG	GLN	Α	220	38.463	10.129	10.659	1.00	26.97	A
	ATOM	1236	CD	GLN	Α	220	38.648	9.343	9.372	1.00	29.95	A
45	ATOM	1237	OE1	GLN	Α	220	37.968	9.590	8.373	1.00	33.12	А
	ATOM	1238	NE2	GLN	Α	220	39.578	8.393	9.389	1.00		А
	ATOM	1239	С			220	39.757	13.610	11.735	1.00		A
	ATOM	1240	0			220	39.609	14.339	10.751	1.00		A
	ATOM	1241	N			221	40.566	13.906	12.746	1.00		A
50	ATOM	1242	CA			221	41.361	15.120	12.753	1.00		A
•	ATOM	1243	СВ			221	41.867	15.416	14.175	1.00		A
	ATOM	1244		ILE			42.764	16.656	14.167	1.00		A
	ATOM	1245		ILE			40.660	15.613	15.102	1.00		A
	ATOM	1245		ILE			41.003	15.613	16.543	1.00		A
55							42.536					
טט	ATOM	1247	C			221		14.996	11.783	1.00		A
	ATOM	1248	O N			221	43.106	13.915	11.613	1.00		A
	ATOM	1249	N			222	42.877	16.101	11.127	1.00		A
	ATOM	1250	CA			222	43.980	16.098	10.174	1.00		A
	ATOM	1251	СВ	THR	А	222	43.470	15.836	8.750	1.00	т9.92	А

	ATOM	1252	OG1	THR	Α	222	44.587	15.637	7.875	1.00	18.78	А
	ATOM	1253	CG2	THR	Α	222	42.630	17.018	8.257	1.00	18.16	A
	ATOM	1254	С	THR	Α	222	44.735	17.428	10.192	1.00	19.60	A
	ATOM	1255	0	THR	Α	222	44.509	18.257	11.084	1.00	18.59	A
5	ATOM	1256	N	ASP	Α	223	45.630	17.610	9.216	1.00	18.69	A
	ATOM	1257	CA	ASP	Α	223	46.440	18.825	9.069	1.00	20.12	A
	ATOM	1258	СВ	ASP	Α	223	45.532	20.065	9.108	1.00	23.51	A
	ATOM	1259	CG	ASP	Α	223	46.248	21.335	8.670	1.00	27.09	A
	ATOM	1260	OD1	ASP	Α	223	47.283	21.227	7.975	1.00	26.28	A
10	ATOM	1261		ASP			45.765	22.438	9.009	1.00	26.15	А
	ATOM	1262	С	ASP	Α	223	47.516	18.913	10.150	1.00	21.73	A
	ATOM	1263	0	ASP	Α	223	47.439	19.751	11.055	1.00	22.76	А
	ATOM	1264	N	PHE	Α	224	48.535	18.063	10.027	1.00	20.75	А
	ATOM	1265	CA	PHE	Α	224	49.611	17.988	11.009	1.00	20.11	A
15	ATOM	1266	СВ	PHE	Α	224	49.805	16.527	11.424	1.00	20.62	A
	ATOM	1267	CG	PHE	Α	224	48.682	15.991	12.263	1.00	21.41	A
	ATOM	1268	CD1	PHE	Α	224	48.598	16.312	13.614	1.00	23.05	А
	ATOM	1269	CD2	PHE	Α	224	47.681	15.212	11.693	1.00	22.27	А
	ATOM	1270	CE1	PHE	Α	224	47.528	15.868	14.389	1.00	23.30	A
20	ATOM	1271	CE2	PHE	Α	224	46.606	14.763	12.457	1.00	21.11	A
	ATOM	1272	CZ	PHE	Α	224	46.530	15.093	13.807	1.00	22.02	A
	ATOM	1273	С	PHE	Α	224	50.957	18.583	10.619	1.00	20.45	А
	ATOM	1274	0	PHE	Α	224	51.905	18.547	11.407	1.00	20.73	А
	ATOM	1275	N	GLY	Α	225	51.049	19.125	9.412	1.00	22.02	А
25	ATOM	1276	CA	GLY	Α	225	52.301	19.713	8.981	1.00	22.66	A
	ATOM	1277	С	GLY	Α	225	52.742	20.822	9.920	1.00	24.99	A
	ATOM	1278	0	GLY	Α	225	53.939	21.041	10.122	1.00	24.52	А
	ATOM	1279	N	THR	Α	226	51.779	21.524	10.508	1.00	23.50	A
	ATOM	1280	CA	THR	Α	226	52.106	22.613	11.416	1.00	25.16	А
30	ATOM	1281	СВ	THR	Α	226	51.199	23.829	11.160		24.76	A
	ATOM	1282	OG1	THR	Α	226	49.831	23.410	11.113	1.00	22.68	A
	ATOM	1283	CG2	THR	Α	226	51.571	24.490	9.834	1.00	25.00	А
	ATOM	1284	С	THR	Α	226	52.046	22.233	12.894	1.00	25.79	A
	ATOM	1285	0	THR	Α	226	52.019	23.100	13.768	1.00	24.54	А
35	ATOM	1286	N	ALA	Α	227	52.037	20.935	13.173	1.00	24.97	A
	ATOM	1287	CA	ALA	Α	227	52.004	20.475	14.550	1.00	25.49	А
	ATOM	1288	СВ	ALA	Α	227	51.659	18.993	14.607	1.00	22.85	А
	ATOM	1289	С	ALA	Α	227	53.384	20.715	15.149		27.70	A
	ATOM	1290	0	ALA	Α	227	54.331	21.047	14.435	1.00	26.60	А
40	ATOM	1291	N	LYS			53.491	20.558	16.461		28.53	А
	ATOM	1292	CA	LYS			54.760	20.745	17.149	1.00	32.12	A
	ATOM	1293	СВ	LYS			54.699	21.974	18.054		33.81	A
	ATOM	1294	CG	LYS	Α	228	56.007	22.294	18.765	1.00	41.23	А
	ATOM	1295	CD	LYS			57.082	22.725	17.768		47.57	А
45	ATOM	1296	CE	LYS			58.401	23.056	18.462	1.00	49.82	А
	ATOM	1297	NZ	LYS			59.459	23.425	17.480		51.49	А
	ATOM	1298	С	LYS	Α	228	55.019	19.504	17.985	1.00	33.25	A
	ATOM	1299	0	LYS			54.190	19.129	18.815		33.70	А
	ATOM	1300	N	VAL			56.159	18.860	17.756		33.64	А
50	ATOM	1301	CA	VAL			56.516	17.661	18.501	1.00	34.66	А
	ATOM	1302	СВ	VAL			57.248	16.646	17.609		33.50	А
	ATOM	1303	CG1	VAL			57.619	15.419	18.415	1.00	32.34	А
	ATOM	1304		VAL			56.370	16.264	16.436		34.25	А
	ATOM	1305	С	VAL			57.420	18.035	19.668		37.57	A
55	ATOM	1306	0	VAL			58.581	18.392	19.474		35.91	A
	ATOM	1307	N	LEU			56.877	17.948	20.878		40.57	А
	ATOM	1308	CA	LEU			57.615	18.289	22.088		46.10	A
	ATOM	1309	СВ			230	56.654	18.417	23.270		44.71	A
	ATOM	1310	CG	LEU			55.627	19.545	23.207		44.50	A

	ATOM	1311	CD1	LEU A 230	54.673	19.430	24.383	1.00 44.39	A
	ATOM	1312	CD2	LEU A 230	56.340	20.885	23.214	1.00 44.81	А
	ATOM	1313	С	LEU A 230		17.279	22.440	1.00 50.42	A
	MOTA	1314	0	LEU A 230	58.603	16.104	22.089	1.00 51.64	A
5	MOTA	1315	N	SER A 231	L 59.717	17.756	23.145	1.00 55.81	A
	ATOM	1316	CA	SER A 231		16.914	23.583	1.00 61.14	А
	ATOM	1317	СВ	SER A 231		17.200	22.750	1.00 61.27	A
	MOTA	1318	OG	SER A 231	L 62.444	18.568	22.823	1.00 62.85	A
	ATOM	1319	С	SER A 231	L 61.124	17.126	25.071	1.00 64.65	A
10	ATOM	1320	0	SER A 231	L 61.392	16.164	25.794	1.00 65.70	А
	ATOM	1321	N	PRO A 232		18.387	25.549	1.00 67.54	A
	ATOM	1322	CD	PRO A 232		19.651	24.823	1.00 68.60	А
	MOTA	1323	CA	PRO A 232	2 61.358	18.655	26.966	1.00 68.74	A
	ATOM	1324	CB	PRO A 232	61.109	20.158	27.086	1.00 68.83	A
15	ATOM	1325	CG	PRO A 232	61.505	20.666	25.737	1.00 68.96	А
10	ATOM	1326	C	PRO A 232		17.846	27.899	1.00 69.17	A
	ATOM	1327	0	PRO A 232		17.494	27.541	1.00 69.94	A
	MOTA	1328	N	ALA A 23	7 57.424	23.198	27.637	1.00 80.06	A
	ATOM	1329	CA	ALA A 23	7 56.783	23.047	26.335	1.00 79.29	A
20	ATOM	1330	СВ	ALA A 23	55.275	22.907	26.512	1.00 78.64	А
	ATOM	1331	C	ALA A 23		24.239	25.433	1.00 79.07	A
	MOTA	1332	0	ALA A 23		25.113	25.249	1.00 79.47	A
	MOTA	1333	N	ALA A 238	58.297	24.280	24.871	1.00 78.57	A
	ATOM	1334	CA	ALA A 238	58.683	25.383	23.992	1.00 78.50	A
25	ATOM	1335	СВ	ALA A 238	60.186	25.347	23.728	1.00 78.50	A
	ATOM	1336	С	ALA A 238		25.327	22.673	1.00 78.15	A
	ATOM	1337	0	ALA A 238		24.341	22.375	1.00 77.96	A
	MOTA	1338	N	ALA A 239		26.393	21.887	1.00 77.28	A
	MOTA	1339	CA	ALA A 239	57.338	26.452	20.603	1.00 76.27	A
30	MOTA	1340	СВ	ALA A 239	55.849	26.489	20.827	1.00 76.61	A
	ATOM	1341	С	ALA A 239		27.667	19.793	1.00 75.38	А
		1342				27.955	19.700	1.00 75.89	
	ATOM		0	ALA A 239					A
	ATOM	1343	N	ASN A 240		28.357	19.214	1.00 73.95	A
	MOTA	1344	CA	ASN A 240	56.967	29.553	18.389	1.00 71.07	A
35	MOTA	1345	CB	ASN A 240	58.151	30.400	18.874	1.00 71.47	A
	ATOM	1346	CG	ASN A 240	59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347		ASN A 240		30.149	16.943	1.00 72.03	A
	ATOM	1348		ASN A 240		29.665	18.964	1.00 71.91	A
	MOTA	1349	С	ASN A 240		29.178	16.928	1.00 69.41	A
40	MOTA	1350	0	ASN A 240	57.480	28.024	16.624	1.00 70.09	A
	MOTA	1351	N	ALA A 241	L 57.055	30.165	16.038	1.00 66.62	A
	ATOM	1352	CA	ALA A 241	L 57.246	30.013	14.585	1.00 63.94	А
	ATOM	1353	C	ALA A 241		30.080	13.772	1.00 60.63	A
	ATOM	1354	0	ALA A 241		30.880	12.845	1.00 61.29	A
45	ATOM	1355	СВ	ALA A 241	L 57.979	28.704	14.246	1.00 65.23	A
	MOTA	1356	N	PHE A 242	2 54.984	29.236	14.113	1.00 56.72	A
	ATOM	1357	CA	PHE A 242	53.712	29.196	13.394	1.00 52.53	A
	ATOM	1358	СВ	PHE A 242		27.767	12.923	1.00 49.14	А
		1359	CG			27.590	12.354	1.00 47.38	
50	ATOM			PHE A 242					A
50	ATOM	1360		PHE A 242		28.067	11.085	1.00 47.69	A
	MOTA	1361	CD2	PHE A 242	2 51.038	26.975	13.102	1.00 45.45	A
	ATOM	1362	CE1	PHE A 242	2 50.445	27.937	10.565	1.00 46.75	A
	ATOM	1363		PHE A 242		26.840	12.594	1.00 45.41	А
		1364	CZ	PHE A 242		27.323	11.322	1.00 46.55	
	ATOM								A
55	ATOM	1365	С	PHE A 242		29.688	14.229	1.00 50.08	А
	ATOM	1366	0	PHE A 242	52.502	29.505	15.444	1.00 49.86	A
	MOTA	1367	N	VAL A 243	51.566	30.305	13.557	1.00 47.67	A
	ATOM	1368	CA	VAL A 243		30.809	14.200	1.00 46.21	A
	ATOM	1369	CB	VAL A 243		32.352	14.258	1.00 47.36	A
	AIOM	T 2 0 2	CD	vAu A 24.	5 50.540	JZ.JJZ	T4.470	1.00 47.30	A

	MOTA	1370	CG1	VAL A	243	4	19.012	32.844	14.825	1.00	47.54	A
	ATOM	1371	CG2	VAL A	243	5	51.497	32.842	15.109	1.00	48.50	A
	ATOM	1372	С	VAL A		4	19.150	30.342	13.389		44.12	A
	ATOM	1373	0	VAL A			18.956	30.765	12.247		44.46	A
5	ATOM	1374	N	GLY A			18.348	29.467	13.985		40.48	A
5	ATOM			GLY A				28.941	13.306		37.65	
		1375	CA				17.176					A
	ATOM	1376	С	GLY A			16.101	29.960	12.964		35.39	A
	MOTA	1377	0	GLY A			16.313	31.168	13.065		35.92	A
	ATOM	1378	N	THR A	. 245	4	14.936	29.463	12.560		33.30	Α
10	MOTA	1379	CA	THR A	. 245	4	13.813	30.312	12.184	1.00	30.20	А
	ATOM	1380	СВ	THR A	245	4	12.593	29.450	11.829	1.00	32.00	Α
	ATOM	1381	OG1	THR A	245	4	12.952	28.573	10.755	1.00	32.81	Α
	ATOM	1382	CG2	THR A	245	4	11.419	30.319	11.390	1.00	28.34	A
	ATOM	1383	С	THR A		4	13.476	31.296	13.296		27.96	Α
15	ATOM	1384	0	THR A			13.212	30.907	14.434		25.46	А
	ATOM	1385	N	ALA A			13.486	32.576	12.938		25.22	A
	ATOM	1386	CA	ALA A			13.247	33.675	13.867		23.27	A
	ATOM	1387	CB	ALA A			12.956	34.955	13.082		22.94	A
20	ATOM	1388	C	ALA A			12.178	33.475	14.934		21.27	A
20	ATOM	1389	0	ALA A			12.431	33.705	16.114		20.93	A
	MOTA	1390	N	GLN A			10.988	33.047	14.536		19.67	A
	MOTA	1391	CA	GLN A			39.911	32.886	15.504		20.17	Α
	ATOM	1392	СВ	GLN	247		88.608	32.535	14.779		21.89	AC1
	ATOM	1393	CG	GLN	247	3	88.522	33.076	13.355	0.50	26.18	AC1
25	MOTA	1394	CD	GLN	247	3	37.220	33.794	13.064	0.50	27.30	AC1
	MOTA	1395	OE1	GLN	247	3	36.172	33.447	13.605	0.50	30.13	AC1
	ATOM	1396	NE2	GLN	247	3	37.278	34.792	12.189	0.50	28.70	AC1
	ATOM	1397	С	GLN A	247	4	10.181	31.849	16.595	1.00	19.43	A
	ATOM	1398	0	GLN A	247	3	39.546	31.883	17.648	1.00	18.93	Α
30	ATOM	1399	N	TYR A			11.132	30.948	16.359		18.60	A
	ATOM	1400	CA	TYR A			11.441	29.896	17.329		19.20	A
	ATOM	1401	СВ	TYR A			11.333	28.529	16.642		17.53	A
	ATOM	1402	CG	TYR A			10.013	28.362	15.927		19.32	A
	ATOM	1403	CD1	TYR A			88.859	28.010	16.625		17.69	A
35												
33	ATOM	1404	CE1				37.617	27.976	15.990		18.18	A
	ATOM	1405	CD2	TYR A			39.897	28.664	14.569		16.87	A
	ATOM	1406	CE2	TYR A			38.665	28.635	13.924		19.17	A
	MOTA	1407	CZ	TYR A			37.527	28.295	14.643		19.46	A
	MOTA	1408	OH	TYR A			36.299	28.311	14.023		18.98	A
40	ATOM	1409	С	TYR A	248	4	12.810	30.039	17.993	1.00	20.42	Α
	MOTA	1410	0	TYR A	248	4	13.208	29.191	18.792	1.00	19.19	A
	ATOM	1411	N	VAL A	249	4	13.523	31.114	17.673	1.00	20.20	A
	ATOM	1412	CA	VAL A	249	4	14.841	31.343	18.251	1.00	20.91	A
	ATOM	1413	СВ	VAL A	249	4	15.542	32.532	17.570	1.00	21.18	A
45	ATOM	1414	CG1	VAL A	249		16.821	32.896	18.317		22.45	Α
	ATOM	1415		VAL A			15.862	32.170	16.139		24.01	A
	ATOM	1416	C	VAL A			14.764	31.606	19.750		21.52	A
	ATOM	1417	0	VAL A			13.915	32.368	20.216		22.72	A
			N				15.654				20.70	
50	ATOM	1418		SER A				30.965	20.503		21.65	A
50	ATOM	1419	CA	SER A			15.697	31.133	21.951			A
	ATOM	1420	СВ	SER A			16.370	29.919	22.613		22.02	A
	MOTA	1421	OG	SER A			17.692	29.725	22.132		22.12	A
	MOTA	1422	С	SER A			16.476	32.402	22.280		22.13	A
	MOTA	1423	0	SER A			17.332	32.828	21.511		22.77	A
55	MOTA	1424	N	PRO A	251	4	16.180	33.029	23.425	1.00	22.23	A
	MOTA	1425	CD	PRO A	251	4	15.163	32.684	24.433	1.00	22.97	A
	MOTA	1426	CA	PRO A	251	4	16.893	34.254	23.800	1.00	22.52	Α
	MOTA	1427	СВ	PRO A			16.233	34.650	25.127	1.00	23.06	A
	ATOM	1428	CG	PRO A			15.726	33.329	25.676		22.55	А

	ATOM	1429	С	PRO A	251	48.414	34.115	23.907	1.00 22.15	A
	ATOM	1430	0	PRO A		49.143	35.047	23.563	1.00 22.62	А
	ATOM	1431	N	GLU A	252	48.901	32.966	24.367	1.00 20.69	A
	ATOM	1432	CA	GLU A		50.347	32.772	24.500	1.00 21.40	A
-										
5	MOTA	1433	СВ	GLU A	252	50.673	31.382	25.071	1.00 20.59	A
	ATOM	1434	CG	GLU A	252	49.993	30.232	24.352	1.00 21.91	A
	ATOM	1435	CD	GLU A		48.691	29.822	25.014	1.00 21.51	А
	MOTA	1436	OE 1	GLU A	252	47.989	30.707	25.550	1.00 21.46	A
	ATOM	1437	OE2	GLU A	252	48.367	28.613	24.993	1.00 20.23	А
10	ATOM	1438	С	GLU A		51.071	32.970	23.167	1.00 22.99	А
10										
	MOTA	1439	0	GLU A	252	52.191	33.480	23.136	1.00 23.17	A
	ATOM	1440	N	LEU A	253	50.441	32.576	22.064	1.00 23.00	А
	ATOM	1441	CA	LEU A		51.068	32.753	20.758	1.00 25.62	A
	MOTA	1442	СВ	LEU A	253	50.277	32.029	19.669	1.00 26.75	A
15	ATOM	1443	CG	LEU A	253	50.743	30.620	19.296	1.00 31.87	A
	ATOM	1444		LEU A		50.433	29.651	20.422	1.00 31.81	А
	ATOM	1445	CD2	LEU A	253	50.044	30.179	18.015	1.00 31.86	A
	ATOM	1446	С	LEU A	253	51.201	34.228	20.371	1.00 26.94	A
	ATOM	1447	0	LEU A		52.107	34.601	19.626	1.00 27.09	А
20										
20	ATOM	1448	N	LEU A		50.297	35.059	20.877	1.00 25.83	A
	ATOM	1449	$^{\rm CA}$	LEU A	254	50.297	36.485	20.564	1.00 27.26	A
	ATOM	1450	СВ	LEU A	2.5.4	48.858	37.006	20.564	1.00 25.84	A
	ATOM	1451	CG	LEU A		47.882	36.290	19.621	1.00 24.69	A
	MOTA	1452	CD1	LEU A	254	46.459	36.724	19.932	1.00 23.64	A
25	ATOM	1453	CD2	LEU A	254	48.236	36.597	18.177	1.00 24.24	A
	ATOM	1454	С	LEU A	254	51.134	37.314	21.537	1.00 30.62	A
	MOTA	1455	0	LEU A		51.633	38.383	21.187	1.00 32.35	A
	ATOM	1456	N	THR A	255	51.292	36.821	22.758	1.00 32.47	A
	ATOM	1457	CA	THR A	255	52.056	37.547	23.759	1.00 36.70	A
30	ATOM	1458	СВ	THR A		51.368	37.478	25.127	1.00 34.51	А
30										
	ATOM	1459	OG1			51.188	36.106	25.494	1.00 35.49	A
	ATOM	1460	CG2	THR A	255	50.013	38.166	25.077	1.00 33.40	A
	ATOM	1461	С	THR A	2.5.5	53.477	37.035	23.910	1.00 40.09	A
	ATOM	1462		THR A		54.430	37.793	23.772	1.00 43.69	A
			0							
35	MOTA	1463	N	GLU A	256	53.617	35.747	24.189	1.00 44.77	A
	ATOM	1464	CA	GLU A	256	54.932	35.144	24.382	1.00 49.15	A
	ATOM	1465	СВ	GLU A		54.866	34.143	25.534	1.00 51.24	A
	ATOM	1466	CG	GLU A		54.514	34.786	26.862	1.00 56.03	A
	MOTA	1467	CD	GLU A	256	54.053	33.780	27.893	1.00 58.83	A
40	ATOM	1468	OE 1	GLU A	256	54.766	32.776	28.107	1.00 62.13	A
	ATOM	1469		GLU A		52.979	33.996	28.494	1.00 60.34	A
	MOTA	1470	С	GLU A	256	55.475	34.456	23.137	1.00 50.09	A
	ATOM	1471	0	GLU A	256	56.616	33.995	23.127	1.00 50.42	A
	ATOM	1472	N	LYS A		54.658	34.389	22.090	1.00 51.21	A
45										
45	ATOM	1473	CA	LYS A		55.064	33.746	20.845	1.00 51.22	A
	MOTA	1474	CB	LYS A	257	56.244	34.502	20.227	1.00 53.28	A
	ATOM	1475	CG	LYS A	2.5.7	56.558	34.125	18.790	1.00 55.19	A
						57.709				
	ATOM	1476	CD	LYS A			34.961	18.253	1.00 57.52	A
	MOTA	1477	CE	LYS A	257	57.952	34.694	16.777	1.00 58.52	A
50	ATOM	1478	NZ	LYS A	257	58.290	33.268	16.515	1.00 60.88	A
	ATOM	1479	С	LYS A		55.467	32.302	21.138	1.00 50.74	А
	ATOM	1480	0	LYS A		56.432	31.790	20.577	1.00 52.26	A
	ATOM	1481	N	SER A	258	54.721	31.654	22.027	1.00 48.07	A
	ATOM	1482	CA	SER A		54.999	30.273	22.402	1.00 46.87	А
55	ATOM	1483	CB	SER A		55.590	30.229	23.812	1.00 48.88	A
55										
	ATOM	1484	OG	SER A		54.741	30.892	24.734	1.00 53.14	A
	MOTA	1485	С	SER A	258	53.735	29.415	22.342	1.00 44.07	A
	ATOM	1486	0	SER A		52.617	29.932	22.417	1.00 44.17	A
	ATOM	1487	N	ALA A	493	53.917	28.105	22.204	1.00 38.30	A

	ATOM	1488	CA	Z\ T. Z\	Ζ.	259	52.793	27.180	22.127	1.00 34	73	Α
	ATOM	1489	CB			259	52.551	26.779	20.684	1.00 34		A
	ATOM	1490	С			259	53.042	25.940	22.977	1.00 34		
												A
-	ATOM	1491	0	ALA			54.172	25.459	23.086	1.00 31		A
5	ATOM	1492	N			260	51.975	25.428	23.579	1.00 28		A
	MOTA	1493	CA			260	52.056	24.244	24.425	1.00 26		A
	MOTA	1494	СВ			260	52.183	24.654	25.892	1.00 26		Α
	ATOM	1495	SG	CYS	Α	260	50.846	25.739	26.469	1.00 32	.91	Α
	MOTA	1496	С	CYS	Α	260	50.786	23.435	24.224	1.00 22	.83	Α
10	ATOM	1497	0	CYS	Α	260	49.892	23.856	23.495	1.00 22	.14	Α
	ATOM	1498	N	LYS	Α	261	50.706	22.277	24.868	1.00 20	.02	Α
	ATOM	1499	CA	LYS	Α	261	49.526	21.434	24.744	1.00 20	.65	Α
	ATOM	1500	СВ	LYS	Α	261	49.619	20.243	25.696	1.00 23	.28	Α
	ATOM	1501	CG	LYS	Α	261	50.716	19.253	25.347	1.00 27	. 4 4	Α
15	ATOM	1502	CD	LYS	Α	261	50.732	18.117	26.350	1.00 29	.98	Α
	ATOM	1503	CE			261	51.922	17.203	26.134	1.00 32		Α
	ATOM	1504	NΖ			261	51.940	16.121	27.153	1.00 33		Α
	ATOM	1505	C			261	48.268	22.229	25.062	1.00 19		A
	ATOM	1506	0			261	47.253	22.092	24.387	1.00 18		A
20	ATOM	1507	N			262	48.358	23.068	26.089	1.00 16		A
20	ATOM	1507	CA			262	47.235	23.883	26.534	1.00 18		A
	ATOM	1509				262	47.233	24.698	27.770	1.00 18		A
			CB						28.421			
	ATOM	1510	OG G			262	46.517	25.258		1.00 22		A
25	ATOM	1511	C			262	46.736	24.811	25.424	1.00 16		A
25	ATOM	1512	0			262	45.591	25.254	25.450	1.00 15		A
	ATOM	1513	N			263	47.595	25.118	24.456	1.00 16		A
	MOTA	1514	CA			263	47.175	25.970	23.347	1.00 16		Α
	ATOM	1515	СВ			263	48.340	26.228	22.382	1.00 18		Α
	MOTA	1516	OG			263	49.402	26.909	23.031	1.00 22		Α
30	ATOM	1517	С	SER	Α	263	46.040	25.257	22.612	1.00 17		Α
	MOTA	1518	0	SER	Α	263	45.099	25.898	22.148	1.00 17	.57	Α
	MOTA	1519	N	ASP	Α	264	46.119	23.928	22.517	1.00 16	.30	Α
	ATOM	1520	CA	ASP	Α	264	45.069	23.166	21.836	1.00 16	.72	Α
	ATOM	1521	СВ	ASP	Α	264	45.483	21.704	21.620	1.00 15	.92	Α
35	ATOM	1522	CG	ASP	Α	264	46.544	21.539	20.548	1.00 17	.93	Α
	ATOM	1523	OD1	ASP	Α	264	46.642	22.412	19.661	1.00 16	.78	Α
	ATOM	1524	OD2	ASP	Α	264	47.265	20.515	20.579	1.00 16	.64	Α
	ATOM	1525	С	ASP			43.773	23.194	22.646	1.00 17		Α
	ATOM	1526	0	ASP			42.681	23.197	22.076	1.00 18		A
40	ATOM	1527	N			265	43.898	23.205	23.974	1.00 15		A
	ATOM	1528	CA			265	42.730	23.232	24.849	1.00 14		A
	ATOM	1529	CB			265	43.147	23.038	26.313	1.00 11		A
	ATOM	1530	CG			265	43.711	21.641	26.621	1.00 14		A
	ATOM	1531		LEU			44.249	21.579	28.052	1.00 13		A
45	ATOM	1531		LEU			42.619	20.603	26.416	1.00 13		
43												A
	ATOM	1533	C			265	41.999	24.557	24.675	1.00 15		A
	ATOM	1534	0			265	40.777	24.620	24.785	1.00 16		A
	ATOM	1535	N			266	42.746	25.622	24.405	1.00 16		A
50	ATOM	1536	CA			266	42.118	26.918	24.184	1.00 16		A
50	ATOM	1537	СВ			266	43.176	28.015	24.023	1.00 17		A
	MOTA	1538	CG			266	42.618	29.326	23.521	1.00 20		A
	ATOM	1539		TRP			42.313	30.490	24.301	1.00 20		A
	ATOM	1540		TRP			41.782	31.459	23.417	1.00 20		Α
	MOTA	1541		TRP			42.435	30.810	25.660	1.00 20		Α
55	ATOM	1542		TRP			42.270	29.631	22.231	1.00 19	.53	Α
	ATOM	1543	NE1	TRP	Α	266	41.769	30.908	22.163	1.00 19	.61	Α
	MOTA	1544	CZ2	TRP	А	266	41.372	32.727	23.850	1.00 20	.90	Α
	MOTA	1545	CZ3	TRP	А	266	42.026	32.073	26.091	1.00 19	.45	Α
	MOTA	1546	CH2	TRP	Α	266	41.501	33.015	25.185	1.00 20	.71	Α

	ATOM	1547	С	TRP A		41.284	26.795	22.913	1.00 17.22	А
	ATOM	1548	0	TRP A	266	40.139	27.240	22.863	1.00 18.03	A
	MOTA	1549	N	ALA A	267	41.863	26.181	21.886	1.00 17.50	A
	ATOM	1550	CA	ALA A	267	41.155	25.990	20.626	1.00 16.16	A
5	ATOM	1551	СВ	ALA A	267	42.050	25.290	19.621	1.00 14.28	A
	ATOM	1552	С	ALA A	267	39.901	25.159	20.891	1.00 16.28	A
	ATOM	1553	0	ALA A	267	38.835	25.436	20.346	1.00 16.46	А
	ATOM	1554	N	LEU A		40.031	24.144	21.739	1.00 16.57	A
	ATOM	1555	CA	LEU A		38.890	23.299	22.084	1.00 17.03	A
10	ATOM	1556	СВ	LEU A		39.292	22.260	23.139	1.00 15.35	A
10	ATOM	1557	CG	LEU A		38.158	21.429	23.754	1.00 19.00	A
	ATOM	1558		LEU A		37.505	20.578	22.678	1.00 16.17	A
	ATOM	1559	CD1	LEU A		38.718	20.537	24.881	1.00 17.49	A
	ATOM	1560	CDZ	LEU A		37.766	24.179	22.628	1.00 17.49	
1.5										A
15	ATOM	1561	0	LEU A		36.603	24.031	22.247	1.00 15.28	A
	ATOM	1562	N	GLY A		38.119	25.099	23.520	1.00 14.34	A
	ATOM	1563	CA	GLY A		37.124	25.989	24.092	1.00 13.39	A
	ATOM	1564	С	GLY A		36.406	26.808	23.031	1.00 14.94	A
	ATOM	1565	0	GLY A		35.193	27.014	23.114	1.00 14.76	A
20	ATOM	1566	N	CYS A		37.146	27.279	22.030	1.00 13.86	A
	ATOM	1567	CA	CYS A		36.539	28.061	20.958	1.00 16.80	A
	ATOM	1568	СВ	CYS A		37.611	28.634	20.023	1.00 15.97	A
	ATOM	1569	SG	CYS A	270	38.751	29.810	20.780	1.00 20.48	A
	ATOM	1570	С	CYS A	270	35.598	27.175	20.140	1.00 17.50	A
25	ATOM	1571	0	CYS A	270	34.516	27.604	19.741	1.00 18.38	A
	ATOM	1572	N	ILE A	271	36.022	25.939	19.887	1.00 16.99	A
	ATOM	1573	CA	ILE A	271	35.221	25.004	19.104	1.00 16.66	A
	ATOM	1574	СВ	ILE A		36.038	23.741	18.778	1.00 16.53	A
	ATOM	1575	CG2	ILE A		35.155	22.694	18.102	1.00 16.34	A
30	ATOM	1576		ILE A		37.222	24.129	17.882	1.00 15.59	A
-	ATOM	1577	CD1			38.239	23.018	17.690	1.00 14.88	A
	ATOM	1578	C	ILE A		33.920	24.626	19.809	1.00 16.74	A
	ATOM	1579	0	ILE A		32.865	24.576	19.179	1.00 17.12	A
	ATOM	1580	N	ILE A		33.990	24.357	21.111	1.00 16.13	A
35	ATOM	1581	CA	ILE A		32.785	24.021	21.862	1.00 18.30	A
33	ATOM	1582	CB	ILE A		33.097	23.747	23.346	1.00 17.77	A
			CG2	ILE A		31.796	23.666	24.152	1.00 17.77	
	MOTA	1583								A
	ATOM	1584	CG1			33.877	22.437	23.481	1.00 19.55	A
40	ATOM	1585	CD1	ILE A		34.446	22.217	24.886	1.00 18.64	A
40	ATOM	1586	C	ILE A		31.824	25.207	21.776	1.00 19.51	A
	ATOM	1587	0	ILE A		30.624	25.037	21.554	1.00 20.44	A
	ATOM	1588	N	TYR A		32.362	26.409	21.947	1.00 18.52	A
	ATOM	1589	CA	TYR A		31.553	27.615	21.881	1.00 20.48	A
	ATOM	1590	СВ	TYR A		32.418	28.847	22.162	1.00 18.98	A
45	ATOM	1591	CG	TYR A		31.663	30.161	22.125	1.00 20.26	A
	ATOM	1592		TYR A		31.229	30.709	20.916	1.00 20.67	A
	ATOM	1593		TYR A		30.536	31.917	20.880	1.00 20.98	A
	ATOM	1594	CD2	TYR A	273	31.383	30.857	23.302	1.00 19.82	A
	MOTA	1595	CE2	TYR A	273	30.691	32.062	23.280	1.00 20.62	A
50	ATOM	1596	CZ	TYR A	273	30.271	32.587	22.067	1.00 21.15	A
	ATOM	1597	OH	TYR A	273	29.588	33.776	22.049	1.00 21.86	A
	ATOM	1598	С	TYR A	273	30.902	27.730	20.507	1.00 21.54	A
	ATOM	1599	0	TYR A		29.719	28.049	20.401	1.00 22.80	А
	ATOM	1600	N	GLN A		31.676	27.454	19.461	1.00 21.05	А
55	ATOM	1601	CA	GLN A		31.176	27.538	18.095	1.00 21.48	А
	ATOM	1602	СВ	GLN A		32.323	27.341	17.097	1.00 21.41	A
	ATOM	1603	CG	GLN A		31.934	27.596	15.645	1.00 23.15	A
	ATOM	1604	CD	GLN A		33.131	27.588	14.706	1.00 24.80	A
	ATOM	1605		GLN A		34.276	27.446	15.139	1.00 22.51	A
		_ = = = =		21		21.270				2.5

	ATOM	1606	NE2	GLN	Α	274	32.870	27.750	13.413	1.00	22.96	А
	ATOM	1607	С	GLN	Α	274	30.076	26.517	17.828	1.00		А
	MOTA	1608	0	GLN	A	274	29.123	26.806	17.108	1.00	20.50	A
	ATOM	1609	N	LEU	Α	275	30.207	25.324	18.403	1.00	21.44	A
5	ATOM	1610	CA	LEU	Α	275	29.196	24.282	18.208	1.00	20.95	A
	ATOM	1611	СВ	LEU	Α	275	29.645	22.958	18.846	1.00	19.11	A
	ATOM	1612	CG	LEU	Α	275	30.775	22.182	18.159	1.00	21.43	A
	ATOM	1613	CD1	LEU	A	275	31.118	20.936	18.963	1.00	17.64	A
	ATOM	1614	CD2	LEU	Α	275	30.342	21.795	16.754	1.00	20.34	A
10	ATOM	1615	С	LEU	Α	275	27.860	24.697	18.815	1.00	21.32	A
	MOTA	1616	0	LEU			26.802	24.461	18.229	1.00		A
	ATOM	1617	N	VAL			27.921	25.322	19.987	1.00		A
	ATOM	1618	CA	VAL			26.724	25.750	20.702	1.00		A
	ATOM	1619	СВ	VAL			27.011	25.882	22.217	1.00		A
15	ATOM	1620		VAL			25.742	26.291	22.957	1.00		А
	ATOM	1621	CG2	VAL			27.550	24.558	22.766	1.00		A
	ATOM	1622	С	VAL			26.127	27.075	20.211	1.00		А
	ATOM	1623	0	VAL			24.910	27.199	20.070	1.00		A
	ATOM	1624	N	ALA			26.983	28.062	19.965	1.00		A
20	ATOM	1625	CA	ALA			26.533	29.374	19.518	1.00		A
	ATOM	1626	СВ	ALA			27.504	30.444	19.999	1.00		A
	ATOM	1627	С	ALA			26.378	29.458	18.005	1.00		А
	MOTA	1628	0	ALA			25.577	30.242	17.502	1.00		A
2.5	ATOM	1629	N	GLY			27.142	28.651	17.280	1.00		A
25	ATOM	1630	CA	GLY			27.062	28.673	15.834	1.00		A
	ATOM	1631	С	GLY			28.163	29.524	15.231	1.00		A
	ATOM	1632	0	GLY			28.374	29.510	14.015	1.00		A
	ATOM	1633	N	LEU			28.866	30.262	16.086	1.00		A
20	ATOM	1634	CA	LEU			29.962	31.130	15.656	1.00		A
30	MOTA	1635	CB	LEU			29.468	32.575	15.500	1.00		A
	ATOM	1636	CG CD1	LEU			28.364	32.899	14.490	1.00		A
	MOTA	1637		LEU LEU			27.922 28.862	34.344	14.684	1.00		A
	ATOM ATOM	1638 1639	CD2	LEU			31.093	32.670 31.116	13.071 16.687	1.00		A A
35	ATOM	1640	0	LEU			30.848	30.994	17.882	1.00		A
33	ATOM	1641	N	PRO			32.349	31.239	16.236	1.00		A
	ATOM	1642	CD	PRO			32.831	31.404	14.855	1.00		A
	ATOM	1643	CA	PRO			33.464	31.239	17.189	1.00		A
	ATOM	1644	CB	PRO			34.692	31.293	16.282	1.00		A
40	ATOM	1645	CG	PRO			34.189	32.020	15.073	1.00		A
70	ATOM	1646	C			280	33.353	32.444	18.137	1.00		A
	ATOM	1647	0			280	32.750	33.457	17.788	1.00		A
	ATOM	1648	N			281	33.939	32.344	19.345	1.00		A
	ATOM	1649	CD			281	34.810	31.223	19.734	1.00		A
45	ATOM	1650	CA			281	33.935	33.375	20.395	1.00		A
	ATOM	1651	СВ			281	34.781	32.751	21.509	1.00		A
	ATOM	1652	CG	PRO			34.749	31.287	21.219	1.00		A
	ATOM	1653	С	PRO			34.481	34.752	20.017	1.00		A
	ATOM	1654	0			281	33.869	35.781	20.317	1.00		А
50	ATOM	1655	N	PHE			35.644	34.763	19.379	1.00	22.17	А
	ATOM	1656	CA	PHE			36.293	36.007	18.998	1.00		А
	ATOM	1657	СВ	PHE			37.765	35.943	19.406	1.00		А
	ATOM	1658	CG	PHE			37.975	35.482	20.822	1.00		А
	ATOM	1659	CD1	PHE			37.806	36.361	21.888	1.00		А
55	MOTA	1660	CD2	PHE	Α	282	38.291	34.151	21.093	1.00	20.72	А
	ATOM	1661		PHE			37.947	35.921	23.206	1.00		А
	MOTA	1662	CE2	PHE	Α	282	38.433	33.702	22.405	1.00		A
	ATOM	1663	CZ	PHE	Α	282	38.261	34.590	23.466	1.00	19.58	A
	ATOM	1664	С	PHE	Α	282	36.169	36.263	17.503	1.00	24.39	A

	ATOM	1665	0	PHE	Α	282	36.802	35.585	16.694	1.00	25.80	A
	ATOM	1666	N	ARG			35.355	37.248	17.142	1 00	24.99	Α
	ATOM	1667	CA	ARG	Α	283	35.141	37.594	15.741	1.00	26.33	A
	ATOM	1668	CB	ARG	Α	283	33.721	37.209	15.316	1.00	28.91	Α
5	ATOM	1669	CG	ARG			33.293	35.808	15.724		30.27	Α
,												
	ATOM	1670	CD	ARG			31.904	35.493	15.188		33.36	А
	ATOM	1671	NE	ARG	Α	283	30.890	36.392	15.733	1.00	32.76	Α
	ATOM	1672	CZ	ARG	Α	283	30.372	36.287	16.952	1.00	34.79	A
	ATOM	1673		ARG			30.767	35.317	17.768		35.77	A
10												
10	MOTA	1674	NH2	ARG			29.458	37.156	17.359		36.12	А
	ATOM	1675	С	ARG	Α	283	35.328	39.096	15.544	1.00	26.47	Α
	ATOM	1676	0	ARG	Α	283	35.029	39.888	16.438	1.00	26.28	Α
	ATOM	1677	N	ALA			35.818	39.486	14.373		26.70	A
	ATOM	1678	CA	ALA			36.033	40.899	14.079		27.84	Α
15	ATOM	1679	CB	ALA	Α	284	37.188	41.442	14.914	1.00	26.24	Α
	ATOM	1680	С	ALA	Α	284	36.327	41.077	12.602	1.00	28.35	Α
	ATOM	1681	0	ALA			36.560	40.101	11.891		29.91	A
	ATOM	1682	N	GLY	Α	285	36.332	42.329	12.153	1.00	29.29	Α
	ATOM	1683	CA	GLY	Α	285	36.577	42.631	10.753	1.00	29.52	Α
20	ATOM	1684	С	GLY	Δ	285	37.893	42.156	10.168	1.00	30.12	Α
20		1685					37.974					
	ATOM		0	GLY				41.862	8.976		30.60	A
	MOTA	1686	N	ASN	Α	286	38.939	42.097	10.983	1.00	28.49	Α
	ATOM	1687	CA	ASN	Α	286	40.231	41.644	10.489	1.00	26.71	Α
	ATOM	1688	СВ	ASN			41.050	42.825	9.945	1 00	26.11	Α
25												
25	ATOM	1689	CG	ASN			41.310	43.900	10.990		27.83	А
	ATOM	1690	OD1	ASN	Α	286	41.877	43.631	12.049	1.00	27.84	Α
	ATOM	1691	ND2	ASN	Α	286	40.908	45.131	10.685	1.00	25.95	Α
	ATOM	1692	С	ASN			40.997	40.924	11.584	1 00	26.03	Α
	ATOM	1693	0	ASN			40.540	40.851	12.723		25.66	А
30	ATOM	1694	N	GLU	Α	287	42.162	40.391	11.239	1.00	24.81	Α
	ATOM	1695	CA	GLU	Α	287	42.965	39.662	12.206	1.00	27.59	A
	ATOM	1696	СВ	GLU			44.145	38.985	11.510		30.17	A
	ATOM	1697	CG	GLU	А	287	43.776	37.632	10.931		38.21	Α
	ATOM	1698	CD	GLU	Α	287	44.900	36.998	10.140	1.00	41.86	Α
35	ATOM	1699	OE 1	GLU	Α	287	46.061	37.036	10.608	1.00	43.08	A
	ATOM	1700		GLU			44.612	36.449	9.052		45.22	A
	ATOM	1701	С	GLU	А	287	43.459	40.485	13.383		25.05	A
	ATOM	1702	0	GLU	Α	287	43.382	40.030	14.521	1.00	26.41	Α
	ATOM	1703	N	TYR	Α	288	43.966	41.685	13.122	1.00	23.04	A
40	ATOM	1704	CA	TYR			44.460	42.528	14.205		22.34	A
40												
	ATOM	1705	СВ	TYR			44.867	43.913	13.691		21.07	Α
	ATOM	1706	CG	TYR	Α	288	45.275	44.858	14.805	1.00	21.07	Α
	ATOM	1707	CD1	TYR	Α	288	46.533	44.762	15.405	1.00	21.23	A
	ATOM	1708		TYR			46.891	45.588	16.475		20.43	A
4.5												
45	ATOM	1709	CD2	TYR	А	288	44.380	45.809	15.302	1.00	22.32	А
	ATOM	1710	CE2	TYR	Α	288	44.725	46.637	16.373	1.00	23.28	Α
	ATOM	1711	CZ	TYR	Δ	288	45.981	46.518	16.953	1.00	22.96	Α
	ATOM	1712	OH	TYR			46.316	47.313	18.024		23.18	A
	MOTA	1713	С	TYR	Α	288	43.402	42.698	15.288	1.00	21.38	Α
50	ATOM	1714	0	TYR	Α	288	43.710	42.616	16.473	1.00	22.09	Α
	ATOM	1715	N	LEU	Α	289	42.159	42.939	14.874	1.00	21.88	Α
	ATOM	1716	CA	LEU			41.055	43.130	15.811		21.98	A
	MOTA	1717	СВ	LEU			39.821	43.673	15.078		22.90	А
	ATOM	1718	CG	LEU	Α	289	39.896	45.130	14.601	1.00	26.52	Α
55	ATOM	1719	CD1	LEU			38.706	45.436	13.696	1.00	26.55	Α
				LEU								
	ATOM	1720					39.914	46.071	15.807		23.13	A
	ATOM	1721	С	LEU			40.686	41.849	16.560		21.24	Α
	MOTA	1722	0	LEU	Α	289	40.256	41.897	17.715	1.00	20.72	Α
	ATOM	1723	N	ILE	А	290	40.843	40.708	15.900		19.62	Α

	MOTA	1724	CA	ILE .	A 290	40.538	39.433	16.533	1.00	18.54	A
	ATOM	1725	СВ	TT.E	A 290	40.560	38.281	15.509	1.00	18 52	А
	ATOM	1726			A 290	40.503	36.934	16.234	1.00		A
	ATOM	1727	CG1	ILE .	A 290	39.378	38.429	14.545	1.00	18.88	A
5	ATOM	1728	CD1	ILE .	A 290	39.421	37.483	13.357	1.00	19 81	А
9											
	MOTA	1729	С		A 290	41.578	39.167	17.618	1.00		A
	MOTA	1730	0	ILE .	A 290	41.236	38.788	18.737	1.00	18.20	A
	ATOM	1731	N	PHE.	A 291	42.849	39.376	17.286	1.00	18.76	A
	ATOM	1732	CA		A 291	43.925	39.156	18.247	1.00		A
10											
10	ATOM	1733	СВ		A 291	45.286	39.434	17.606	1.00	20.71	A
	ATOM	1734	CG	PHE .	A 291	45.644	38.480	16.503	1.00	22.92	A
	ATOM	1735	CD1		A 291	45.065	37.214	16.443	1.00		А
	MOTA	1736			A 291	46.588	38.830	15.543	1.00		A
	MOTA	1737	CE1	PHE .	A 291	45.423	36.310	15.440	1.00	24.51	A
15	ATOM	1738	CE2	PHE .	A 291	46.954	37.931	14.535	1.00	25.54	A
	ATOM	1739	CZ		A 291	46.370	36.670	14.485	1.00		А
	ATOM	1740	С	PHE.	A 291	43.739	40.061	19.451	1.00		A
	MOTA	1741	0	PHE .	A 291	43.992	39.671	20.593	1.00	22.32	A
	ATOM	1742	N	GT ₁ N	A 292	43.284	41.275	19.178	1.00	23.27	А
20		1743			A 292		42.264	20.216	1.00		
20	ATOM		CA			43.055					A
	ATOM	1744	СВ	GLN .	A 292	42.574	43.559	19.562	1.00	25.77	A
	ATOM	1745	CG	GLN .	A 292	42.577	44.773	20.447	1.00	28.45	A
	ATOM	1746	CD		A 292	42.469	46.057	19.638	1.00		А
	MOTA	1747		GLN .		41.520	46.244	18.872	1.00		A
25	ATOM	1748	NE2	GLN .	A 292	43.449	46.944	19.799	1.00	27.61	A
	ATOM	1749	С	GLN .	A 292	42.018	41.733	21.204	1.00	22.97	A
	ATOM	1750	0		A 292	42.200	41.832	22.415	1.00		A
	ATOM	1751	N	LYS .	A 293	40.937	41.154	20.687	1.00		A
	MOTA	1752	CA	LYS .	A 293	39.895	40.612	21.558	1.00	22.18	A
30	ATOM	1753	СВ	LYS	A 293	38.664	40.223	20.740	1.00	22.69	А
50		1754									A
	MOTA		CG		A 293	37.919	41.407	20.153	1.00		
	ATOM	1755	CD	LYS .	A 293	36.651	40.961	19.429	1.00	27.88	A
	ATOM	1756	CE	LYS .	A 293	35.857	42.161	18.926	1.00	30.85	A
	ATOM	1757	ΝZ		A 293	34.612	41.750	18.214	1.00		А
25											
35	ATOM	1758	С		A 293	40.398	39.398	22.343	1.00		A
	ATOM	1759	0	LYS .	A 293	40.041	39.204	23.509	1.00	22.01	A
	ATOM	1760	N	TLE	A 294	41.226	38.583	21.702	1.00	19.91	A
	ATOM	1761	CA		A 294	41.774	37.394	22.347	1.00		A
	ATOM	1762	СВ		A 294	42.631	36.575	21.349	1.00		A
40	ATOM	1763	CG2	ILE .	A 294	43.481	35.550	22.098	1.00	17.70	A
	ATOM	1764	CG1	ILE .	A 294	41.716	35.897	20.318	1.00	17.93	А
	ATOM	1765	CD1		A 294	42.467	35.237	19.178	1.00		
											A
	MOTA	1766	С		A 294	42.618	37.727	23.587	1.00		A
	MOTA	1767	0	ILE .	A 294	42.366	37.199	24.673	1.00	20.86	A
45	ATOM	1768	N	TLE	A 295	43.610	38.600	23.439	1.00	21.88	А
						44.461					
	MOTA	1769	CA		A 295		38.934	24.582	1.00		A
	ATOM	1770	СВ	ILE .	A 295	45.668	39.805	24.175	1.00	23.93	A
	ATOM	1771	CG2	ILE .	A 295	46.514	39.066	23.140	1.00	24.61	A
	ATOM	1772	CG1	TTE	A 295	45.189	41.151	23.637	1.00		А
50											
50	MOTA	1773	CDI		A 295	46.317	42.149	23.433	1.00		A
	ATOM	1774	С	ILE .	A 295	43.720	39.636	25.717	1.00	24.80	A
	ATOM	1775	0	ILE	A 295	44.214	39.687	26.842	1.00	24.76	А
	ATOM	1776	N		A 296	42.539	40.173	25.425	1.00		A
	MOTA	1777	CA		A 296	41.743	40.853	26.444	1.00		A
55	ATOM	1778	СВ	LYS .	A 296	41.178	42.170	25.894	1.00	27.39	A
	ATOM	1779	CG		A 296	42.240	43.141	25.413	1.00		А
	ATOM	1780	CD		A 296	41.634	44.410	24.826	1.00		A
	ATOM	1781	CE		A 296	41.009	45.283	25.900	1.00	39.29	A
	ATOM	1782	NZ	LYS .	A 296	40.564	46.603	25.357	1.00	41.72	A

	ATOM	1783	С	LYS	A	296	40.593	39.958	26.893	1.00	25.50	А
	ATOM	1784	0	LYS	Α	296	39.770	40.361	27.713		24.02	А
	ATOM	1785	N	LEU	A	297	40.550	38.742	26.349	1.00	25.67	A
	ATOM	1786	CA	LEU	Α	297	39.500	37.777	26.666	1.00	25.16	A
5	ATOM	1787	СВ	LEU	Α	297	39.632	37.285	28.111	1.00	24.80	A
	ATOM	1788	CG	LEU	Α	297	38.766	36.068	28.460	1.00	26.43	A
	ATOM	1789	CD1	LEU	Α	297	39.238	34.852	27.646	1.00	26.70	A
	ATOM	1790	CD2	LEU	A	297	38.856	35.777	29.951	1.00	24.84	A
	ATOM	1791	С	LEU	Α	297	38.151	38.459	26.467	1.00	25.11	A
10	ATOM	1792	0	LEU	Α	297	37.261	38.378	27.309		25.28	A
	MOTA	1793	N	GLU			38.007	39.127	25.331		24.98	A
	ATOM	1794	CA	GLU			36.786	39.847	25.023		25.31	A
	ATOM	1795	СВ	GLU			37.143	41.139	24.291		27.13	A
	ATOM	1796	CG	GLU			35.991	42.092	24.108		31.28	A
15	ATOM	1797	CD	GLU			36.419	43.362	23.410		34.40	A
	ATOM	1798		GLU			37.348	44.027	23.918		35.90	A
	ATOM	1799		GLU			35.832	43.693	22.359		36.16	A
	ATOM	1800	С	GLU			35.766	39.057	24.207		23.79	A
•	ATOM	1801	0	GLU			35.832	39.017	22.979		24.35	A
20	ATOM	1802	N	TYR			34.825	38.427	24.902		23.45	A
	ATOM	1803	CA	TYR			33.760	37.663	24.265		23.98	A
	ATOM	1804	СВ	TYR			34.264	36.304	23.755		20.13	A
	ATOM	1805	CG	TYR			34.348	35.233	24.828		21.17	A
25	ATOM	1806		TYR TYR			35.336	35.279	25.810		19.32	A
23	ATOM	1807					35.389	34.332 34.201	26.826		19.30 18.96	A
	MOTA	1808 1809	CD2	TYR			33.410 33.456	33.243	24.888 25.907			A
	ATOM		CE2								19.41	A
	ATOM ATOM	1810 1811	CZ OH	TYR TYR			34.449 34.511	33.321 32.401	26.870 27.881		18.79 18.77	A A
30	ATOM	1812	C	TYR			32.699	37.437	25.331		25.20	A
30	ATOM	1813	0	TYR			32.942	37.437	26.506		26.46	A
	ATOM	1814	N	ASP			31.522	36.981	24.927		26.94	A
	ATOM	1815	CA	ASP			30.467	36.710	25.891		30.60	A
	ATOM	1816	CB	ASP			29.665	37.981	26.179		35.86	A
35	ATOM	1817	CG	ASP			29.228	38.687	24.923		42.04	A
	ATOM	1818		ASP			28.450	38.088	24.149		45.98	A
	ATOM	1819		ASP			29.666	39.840	24.707		45.69	A
	ATOM	1820	С	ASP			29.564	35.608	25.363		29.26	A
	ATOM	1821	0	ASP			29.590	35.299	24.172		28.64	А
40	ATOM	1822	N	PHE			28.778	35.011	26.253		28.96	А
	ATOM	1823	CA	PHE	Α	301	27.884	33.924	25.871	1.00	30.48	A
	ATOM	1824	СВ	PHE	Α	301	27.818	32.854	26.968	1.00	29.17	A
	ATOM	1825	CG	PHE	Α	301	29.147	32.279	27.356	1.00	29.29	A
	ATOM	1826	CD1	PHE	Α	301	29.978	32.949	28.245	1.00	27.31	A
45	ATOM	1827	CD2	PHE	Α	301	29.560	31.050	26.845	1.00	27.89	A
	ATOM	1828	CE1	PHE	Α	301	31.205	32.403	28.625	1.00	28.83	A
	MOTA	1829	CE2	PHE	Α	301	30.781	30.498	27.217	1.00	28.05	A
	ATOM	1830	CZ	PHE	Α	301	31.605	31.175	28.110	1.00	28.27	A
	ATOM	1831	С			301	26.459	34.384	25.619		32.20	A
50	ATOM	1832	0			301	25.946	35.261	26.317		32.36	A
	ATOM	1833	N	PRO			25.798	33.804	24.607		33.29	A
	ATOM	1834	CD	PRO			26.313	32.943	23.529		34.04	A
	ATOM	1835	CA	PRO			24.415	34.199	24.341		35.24	A
	ATOM	1836	СВ	PRO			24.144	33.608	22.959		34.01	A
55	ATOM	1837	CG	PRO			25.041	32.413	22.921		35.48	A
	ATOM	1838	C	PRO			23.567	33.561	25.444		37.39	A
	ATOM	1839	0	PRO			23.935	32.518	25.986		38.49	A
	ATOM	1840	N	ALA			22.447	34.188	25.783		39.36	A
	ATOM	1841	CA	ALA	А	3 ∪3	21.572	33.692	26.843	T.00	40.65	А

	ATOM	1842	СВ	ALA	Α	303	20.280	34.506	26.862	1.00	41.66	A
	ATOM	1843	С	ALA	Α	303	21.238	32.197	26.814	1.00	41.25	A
	ATOM	1844	0	ALA	Α	303	21.253	31.537	27.854	1.00	43.16	A
	ATOM	1845	N	ALA	Α	304	20.945	31.665	25.631	1.00	41.04	A
5	ATOM	1846	CA	ALA	Α	304	20.569	30.258	25.480	1.00	40.66	A
	ATOM	1847	СВ	ALA	Α	304	20.121	30.004	24.040	1.00	41.36	A
	ATOM	1848	С	ALA	Α	304	21.628	29.223	25.876	1.00	39.61	A
	ATOM	1849	0	ALA	Α	304	21.298	28.156	26.395	1.00	40.61	A
	ATOM	1850	N	PHE	Α	305	22.891	29.543	25.617	1.00	36.21	A
10	ATOM	1851	CA	PHE	Α	305	24.022	28.662	25.909	1.00	32.08	A
	ATOM	1852	СВ	PHE	A	305	25.259	29.519	26.187	1.00	29.46	A
	ATOM	1853	CG	PHE	Α	305	26.536	28.917	25.690	1.00	28.15	A
	ATOM	1854	CD1	PHE	Α	305	27.146	27.875	26.377	1.00	26.20	A
	ATOM	1855	CD2	PHE	Α	305	27.127	29.386	24.521	1.00	27.05	А
15	ATOM	1856	CE1	PHE	Α	305	28.330	27.308	25.908	1.00	26.92	Α
	ATOM	1857	CE2	PHE	Α	305	28.312	28.826	24.042		26.62	Α
	ATOM	1858	CZ	PHE	Α	305	28.914	27.786	24.737	1.00	26.61	А
	ATOM	1859	С			305	23.811	27.664	27.057		30.09	Α
	ATOM	1860	0	PHE			23.518	28.051	28.187		31.51	А
20	ATOM	1861	N	PHE			23.964	26.378	26.758		27.01	A
	ATOM	1862	CA	PHE			23.801	25.334	27.769		26.30	A
	ATOM	1863	СВ	PHE			24.157	23.970	27.170		25.03	A
	ATOM	1864	CG	PHE			23.548	23.725	25.815		27.24	A
	ATOM	1865		PHE			22.170	23.831	25.622		28.40	A
25	ATOM	1866		PHE			24.350	23.386	24.728		27.84	A
	ATOM	1867		PHE			21.601	23.603	24.365		28.05	A
	ATOM	1868		PHE			23.792	23.155	23.465		28.31	A
	ATOM	1869	CZ	PHE			22.415	23.263	23.283		28.00	A
20	ATOM	1870	C	PHE			24.711	25.652	28.961		26.23	A
30	ATOM	1871	0	PHE			25.927	25.775	28.811		25.59	A
	ATOM	1872	N	PRO			24.125	25.796	30.163		26.67	A
	ATOM	1873	CD	PRO			22.685	25.625	30.430		27.95	A
	ATOM	1874	CA	PRO			24.842	26.110	31.405		26.59	A
25	ATOM	1875	CB	PRO			23.795	25.832	32.481		26.14	A
35	ATOM	1876	CG	PRO			22.531	26.250	31.803		27.86	A
	ATOM	1877	С	PRO			26.145	25.355 25.964	31.659		25.58	A
	ATOM	1878 1879	O	PRO LYS			27.189		31.900		22.65	A
	ATOM ATOM	1880	N CA	LYS			26.085 27.274	24.031 23.232	31.620 31.867		23.91	A A
40	ATOM	1881	CB	LYS			26.887	21.760	32.024		23.25	A
40	ATOM	1882	CG	LYS			26.062	21.532	33.285		28.49	A
	ATOM	1883	CD	LYS			25.618	20.093	33.466		30.17	A
	ATOM	1884	CE	LYS			24.760	19.973	34.722		33.12	A
	ATOM	1885	NZ	LYS			24.122	18.636	34.860		34.13	A
45	ATOM	1886	C	LYS			28.314	23.426	30.769		22.84	A
15	ATOM	1887	0	LYS			29.514	23.411	31.042		22.46	A
	ATOM	1888	N	ALA			27.861	23.621	29.534		21.59	A
	ATOM	1889	CA	ALA			28.792	23.848	28.432		20.02	A
	ATOM	1890	СВ	ALA			28.056	23.856	27.106		18.80	A
50	ATOM	1891	С	ALA			29.481	25.191	28.662		21.41	А
	ATOM	1892	0	ALA			30.680	25.335	28.427		21.39	А
	ATOM	1893	N	ARG			28.717	26.179	29.121		21.39	А
	ATOM	1894	CA	ARG			29.290	27.494	29.388		22.02	А
	ATOM	1895	СВ	ARG			28.213	28.479	29.854		22.39	А
55	ATOM	1896	CG	ARG			28.806	29.756	30.436		25.30	A
	ATOM	1897	CD	ARG			27.780	30.852	30.664		28.33	A
	ATOM	1898	NE	ARG	А	310	28.420	32.039	31.230	1.00	30.18	A
	ATOM	1899	CZ	ARG			27.901	33.263	31.203		32.07	A
	ATOM	1900	NH1	ARG	Α	310	26.719	33.477	30.634	1.00	31.19	А

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	MOTA	1901	NH2	ARG I	A 310	28.567	34.277	31.742	1.00 30	.49	A
	ATOM	1902	С	ARG	A 310	30.376	27.388	30.458	1.00 21	. 65	A
	ATOM	1903				31.464	27.949	30.311	1.00 20		
			0		A 310						A
	ATOM	1904	N	ASP A	A 311	30.074	26.677	31.541	1.00 19	. 57	A
5	ATOM	1905	CA	ASP 2	A 311	31.043	26.512	32.615	1.00 20	. 18	A
		1906				30.460			1.00 20		
	ATOM		СВ		A 311		25.649	33.739			A
	ATOM	1907	CG	ASP A	A 311	31.439	25.446	34.881	1.00 23	.35	Α
	ATOM	1908	OD1	ASP Z	A 311	32.158	24.428	34.885	1.00 24	.91	A
	ATOM	1909	OD 2	ZQP :	A 311	31.500	26.312	35.776	1.00 26	96	A
10											
10	MOTA	1910	С		A 311	32.322	25.877	32.073	1.00 19		A
	ATOM	1911	0	ASP A	A 311	33.422	26.289	32.439	1.00 19	.30	A
	ATOM	1912	N	LEU Z	A 312	32.179	24.891	31.188	1.00 16	. 32	A
	ATOM	1913	CA		A 312	33.349	24.226	30.611	1.00 16		A
	MOTA	1914	СВ		A 312	32.927	23.035	29.744	1.00 16	.12	A
15	ATOM	1915	CG	LEU Z	A 312	34.050	22.320	28.974	1.00 14	.73	A
	ATOM	1916	CD1	LEU Z	A 312	35.192	21.935	29.912	1.00 14	. 56	A
	ATOM	1917		LEU Z		33.477	21.084	28.289	1.00 14		A
	ATOM	1918	С	LEU A	A 312	34.181	25.189	29.774	1.00 16	.61	A
	ATOM	1919	0	LEU Z	A 312	35.402	25.241	29.910	1.00 16	.20	A
20	ATOM	1920	N	VAT.	A 313	33.515	25.949	28.908	1.00 16	20	A
		1921			A 313	34.207			1.00 15		
	ATOM		CA				26.907	28.058			A
	ATOM	1922	СВ	VAL Z	A 313	33.216	27.648	27.130	1.00 16	.42	A
	ATOM	1923	CG1	VAL Z	A 313	33.915	28.796	26.426	1.00 16	.93	A
	ATOM	1924			A 313	32.644	26.672	26.103	1.00 17		A
25											
25	ATOM	1925	С		A 313	34.960	27.923	28.911	1.00 17		A
	MOTA	1926	0	VAL 2	A 313	36.093	28.294	28.591	1.00 18	.00	A
	ATOM	1927	N	GLU Z	A 314	34.342	28.364	30.004	1.00 17	.61	A
	ATOM	1928	CA		A 314	34.986	29.331	30.885	1.00 20		A
	ATOM	1929	СВ	GLU A	A 314	34.009	29.816	31.959	1.00 22	.14	A
30	ATOM	1930	CG	GLU Z	A 314	32.800	30.550	31.396	1.00 26	.52	A
	ATOM	1931	CD	GLU 2	A 314	31.852	31.025	32.478	1.00 31	.26	A
	ATOM	1932	OE1			31.580	30.246		1.00 33		
								33.417			A
	ATOM	1933	OE2	GLU Z	A 314	31.370	32.173	32.387	1.00 34	.81	A
	ATOM	1934	С	GLU Z	A 314	36.217	28.721	31.539	1.00 19	.15	A
35	ATOM	1935	0		A 314	37.134	29.433	31.934	1.00 21		A
55		1936				36.245			1.00 19		
	ATOM		N		A 315		27.400	31.651			A
	ATOM	1937	CA	LYS Z	A 315	37.394	26.749	32.258	1.00 19	.17	A
	ATOM	1938	CB	LYS Z	A 315	36.946	25.514	33.043	1.00 18	.84	A
	ATOM	1939	CG		A 315	36.280	25.885	34.368	1.00 19	62	A
40					A 315				1.00 19		
40	ATOM	1940	CD			35.653	24.696	35.073			A
	ATOM	1941	CE	LYS	315	35.070	25.095	36.427	0.50 21	.00	AC1
	ATOM	1942	NZ	LYS	315	36.119	25.552	37.381	0.50 19	.53	AC1
	ATOM	1943	С		A 315	38.452	26.393	31.218	1.00 18		A
							25.873				
	ATOM	1944	0		A 315	39.511		31.561	1.00 19		A
45	MOTA	1945	Ν	LEU A	A 316	38.164	26.691	29.950	1.00 17	.08	A
	ATOM	1946	CA	LEU A	A 316	39.102	26.429	28.854	1.00 16	.41	A
	ATOM	1947	СВ		A 316	38.414	25.636	27.738	1.00 13		A
	ATOM	1948	CG		A 316	38.028	24.201	28.115	1.00 14		A
	MOTA	1949	CD1	LEU Z	A 316	37.139	23.597	27.031	1.00 12	.38	A
50	ATOM	1950	CD2	LEU 2	A 316	39.302	23.373	28.309	1.00 12	.77	A
	ATOM	1951	C			39.652			1.00 17		
					A 316		27.743	28.290			A
	ATOM	1952	0		A 316	40.851	27.860	28.023	1.00 16		A
	ATOM	1953	N	LEU Z	A 317	38.780	28.729	28.105	1.00 16	.27	A
	ATOM	1954	CA		A 317	39.228	30.022	27.596	1.00 17		A
55											
55	ATOM	1955	СВ		A 317	38.083	30.752	26.887	1.00 16		A
	ATOM	1956	CG	LEU Z	A 317	37.448	29.973	25.727	1.00 18	.81	A
	ATOM	1957	CD1	LEU Z	A 317	36.415	30.851	25.018	1.00 16	. 47	A
	ATOM	1958			A 317	38.528	29.526	24.741	1.00 17		A
	MOTA	1959	С	теО т	A 317	39.745	30.841	28.774	1.00 18	. 4 /	A

	ATOM	1960	0	LEU	Α	317	39.078	31.753	29.273	1.00 18.58	А
	ATOM	1961	N	VAL	Α	318	40.937	30.475	29.229	1.00 18.02	A
	ATOM	1962	CA	VAL	Α	318	41.593	31.141	30.342	1.00 18.85	A
	ATOM	1963	СВ	VAL	Α	318	41.846	30.153	31.500	1.00 19.91	A
5	ATOM	1964	CG1	VAL	Α	318	42.590	30.848	32.634	1.00 20.01	A
	ATOM	1965	CG2	VAL	Α	318	40.520	29.584	31.990	1.00 19.44	A
	ATOM	1966	С	VAL	Α	318	42.923	31.657	29.811	1.00 19.67	А
	ATOM	1967	0	VAL	A	318	43.690	30.902	29.208	1.00 18.26	А
	ATOM	1968	N	LEU	Α	319	43.197	32.939	30.028	1.00 20.07	А
10	ATOM	1969	CA	LEU	А	319	44.436	33.533	29.538	1.00 20.98	А
	ATOM	1970	СВ	LEU			44.521	35.002	29.968	1.00 21.64	А
	ATOM	1971	CG	LEU	А	319	43.418	35.908	29.408	1.00 24.38	А
	ATOM	1972	CD1	LEU			43.606	37.332	29.935	1.00 23.28	А
	ATOM	1973		LEU			43.453	35.887	27.875	1.00 24.33	А
15	ATOM	1974	С	LEU	Α	319	45.680	32.774	29.994	1.00 20.38	А
	ATOM	1975	0	LEU	Α	319	46.568	32.496	29.192	1.00 21.34	А
	ATOM	1976	N	ASP	Α	320	45.742	32.440	31.280	1.00 20.22	А
	ATOM	1977	CA	ASP	Α	320	46.879	31.707	31.833	1.00 20.90	А
	ATOM	1978	СВ	ASP			46.842	31.760	33.365	1.00 20.76	А
20	ATOM	1979	CG	ASP	Α	320	48.049	31.102	34.004	1.00 21.51	А
	ATOM	1980	OD1	ASP	Α	320	48.669	30.226	33.367	1.00 23.46	A
	ATOM	1981		ASP			48.371	31.450	35.159	1.00 23.89	А
	ATOM	1982	С	ASP	Α	320	46.814	30.247	31.367	1.00 20.06	А
	ATOM	1983	0	ASP	Α	320	45.988	29.476	31.840	1.00 20.54	А
25	ATOM	1984	N	ALA	Α	321	47.700	29.876	30.451	1.00 20.68	A
	ATOM	1985	CA	ALA	Α	321	47.733	28.522	29.903	1.00 22.04	A
	ATOM	1986	СВ	ALA	Α	321	48.860	28.411	28.881	1.00 20.75	A
	ATOM	1987	С	ALA	Α	321	47.858	27.400	30.940	1.00 21.62	A
	ATOM	1988	0	ALA	Α	321	47.482	26.259	30.665	1.00 21.99	A
30	ATOM	1989	N	THR	Α	322	48.372	27.715	32.127	1.00 20.89	A
	ATOM	1990	CA	THR	A	322	48.531	26.698	33.167	1.00 20.82	A
	ATOM	1991	СВ	THR	Α	322	49.670	27.051	34.146	1.00 19.47	A
	ATOM	1992	OG1	THR	Α	322	49.341	28.253	34.848	1.00 20.19	A
	ATOM	1993	CG2	THR	Α	322	50.981	27.249	33.394	1.00 21.59	A
35	ATOM	1994	С	THR	Α	322	47.264	26.498	33.983	1.00 19.55	A
	MOTA	1995	0	THR	A	322	47.235	25.673	34.894	1.00 21.13	A
	ATOM	1996	N	LYS	Α	323	46.216	27.248	33.661	1.00 19.33	A
	ATOM	1997	CA	LYS	A	323	44.962	27.122	34.392	1.00 21.20	A
	ATOM	1998	СВ	LYS	Α	323	44.580	28.460	35.030	1.00 23.75	A
40	ATOM	1999	CG	LYS	Α	323	45.562	28.933	36.084	1.00 28.45	A
	ATOM	2000	CD	LYS	Α	323	45.055	30.177	36.799	1.00 33.76	A
	MOTA	2001	CE	LYS	Α	323	46.087	30.678	37.802	1.00 36.15	A
	ATOM	2002	NZ	LYS	Α	323	46.532	29.569	38.693	1.00 37.34	A
	ATOM	2003	С	LYS			43.806	26.614	33.539	1.00 20.68	A
45	ATOM	2004	0	LYS	Α	323	42.649	26.757	33.915	1.00 20.42	A
	ATOM	2005	N	ARG			44.114	26.019	32.392	1.00 19.97	A
	MOTA	2006	CA	ARG			43.060	25.494	31.531	1.00 17.98	A
	ATOM	2007	СВ	ARG			43.461	25.609	30.061	1.00 15.95	A
	ATOM	2008	CG	ARG			43.534	27.050	29.603	1.00 17.34	A
50	ATOM	2009	CD	ARG			43.996	27.194	28.172	1.00 19.80	A
	ATOM	2010	NE	ARG			44.438	28.565	27.944	1.00 16.93	А
	ATOM	2011	CZ	ARG			45.410	28.908	27.108	1.00 19.88	A
	ATOM	2012		ARG			46.045	27.978	26.398	1.00 14.58	A
	ATOM	2013		ARG			45.774	30.181	27.015	1.00 16.51	A
55	ATOM	2014	С	ARG			42.762	24.046	31.883	1.00 18.32	A
	ATOM	2015	0	ARG			43.673	23.222	32.006	1.00 18.20	A
	ATOM	2016	N	LEU			41.479	23.748	32.055	1.00 18.32	A
	ATOM	2017	CA	LEU			41.050	22.403	32.395	1.00 17.79	A
	ATOM	2018	СВ	LEU	А	325	39.523	22.335	32.425	1.00 17.03	A

	ATOM	2019	CG	LEU	Α	325	38.896	21.125	33.116	1.00	15.91	Α
	ATOM	2020	CD1	LEU	Δ.	325	39.392	21.048	34.557	1.00	15 93	Α
	ATOM	2021		LEU			37.375	21.255	33.084	1.00		A
	ATOM	2022	С	LEU	Α	325	41.599	21.433	31.356	1.00	18.68	Α
5	ATOM	2023	0	LEU	Δ	325	41.347	21.586	30.157	1.00	18 28	A
,												
	ATOM	2024	N	GLY			42.354	20.439	31.821	1.00		A
	ATOM	2025	CA	$\operatorname{GL} Y$	Α	326	42.931	19.462	30.915	1.00	16.36	Α
	ATOM	2026	С	GLY	A	326	44.443	19.558	30.807	1.00	19.15	Α
	ATOM	2027	0	GLY			45.093	18.592	30.404	1.00		A
1.0												
10	ATOM	2028	N	CYS	А	327	45.016	20.708	31.161	1.00	18.16	А
	ATOM	2029	CA	CYS	Α	327	46.463	20.867	31.075	1.00	19.30	Α
	ATOM	2030	СВ	CYS	Δ	327	46.856	22.350	31.058	1.00	20.22	Α
		2031							32.649			
	ATOM		SG	CYS			46.782	23.200		1.00		A
	MOTA	2032	С	CYS	Α	327	47.169	20.157	32.228	1.00	20.22	Α
15	ATOM	2033	0	CYS	Α	327	46.561	19.828	33.246	1.00	17.92	Α
	ATOM	2034	N	GLU			48.463	19.933	32.053	1.00		Α
	ATOM	2035	CA	GLU			49.274	19.244	33.042	1.00		A
	ATOM	2036	CB	GLU	Α	328	50.710	19.139	32.507	1.00	28.68	Α
	ATOM	2037	CG	GLU	Α	328	50.754	18.367	31.175	1.00	38.24	Α
20	ATOM	2038	CD	GLU			52.067	18.500	30.414	1.00		A
20												
	ATOM	2039		GLU			52.535	19.643	30.218	1.00		Α
	ATOM	2040	OE2	GLU	Α	328	52.618	17.459	29.991	1.00	44.90	Α
	ATOM	2041	С	GLU	Α	328	49.234	19.876	34.435	1.00	22.11	Α
							49.147	19.161				
	ATOM	2042	0	GLU					35.437	1.00		A
25	ATOM	2043	N	GLU	Α	329	49.276	21.204	34.506	1.00	18.40	Α
	ATOM	2044	CA	GLU	Α	329	49.248	21.875	35.801	1.00	20.13	Α
	ATOM	2045	СВ	GLU	Δ	329	49.587	23.363	35.657	1.00	20 36	Α
	ATOM	2046	CG	GLU			51.014	23.651	35.190	1.00		A
	MOTA	2047	CD	GLU	Α	329	51.191	23.518	33.688	1.00	25.93	Α
30	ATOM	2048	OE1	GLU	Α	329	50.213	23.154	32.995	1.00	26.61	Α
	ATOM	2049		GLU			52.311	23.781	33.198	1.00		A
	ATOM	2050	С	GLU			47.890	21.718	36.480	1.00		A
	ATOM	2051	0	GLU	Α	329	47.775	21.879	37.694	1.00	18.74	Α
	ATOM	2052	N	MET	Α	330	46.863	21.415	35.691	1.00	17.28	A
35		2053		MET			45.520	21.220	36.229	1.00		
33	ATOM		CA									A
	MOTA	2054	СВ	MET	Α	330	44.474	21.833	35.294	1.00	17.65	Α
	ATOM	2055	CG	MET	Α	330	44.460	23.365	35.311	1.00	22.95	Α
	ATOM	2056	SD	MET	Δ	330	44.186	24.026	36.979	1.00	26 78	Α
	ATOM	2057	CE	MET			42.435	23.712	37.186	1.00		Α
40	ATOM	2058	С	MET	Α	330	45.257	19.730	36.422	1.00	14.30	Α
	ATOM	2059	0	MET	Α	330	44.127	19.304	36.629	1.00	15.39	A
	ATOM	2060	N	GLU			46.327	18.949	36.346	1.00	15 60	Α
	ATOM	2061	CA	GLU			46.289	17.501	36.531	1.00		A
	MOTA	2062	СВ	GLU	Α	331	45.607	17.155	37.862	1.00	17.00	Α
45	ATOM	2063	CG	GLU	Α	331	46.070	18.027	39.038	1.00	17.46	Α
	ATOM	2064	CD	GLU			47.591	18.179	39.145	1.00		Α
	ATOM	2065		GLU			48.034	19.073	39.896	1.00	21.39	A
	MOTA	2066	OE2	GLU	Α	331	48.345	17.420	38.500	1.00	18.87	A
	ATOM	2067	С	GLU	Α	331	45.697	16.658	35.398	1.00	17.80	Α
50	ATOM	2068		GLU			45.107	15.602	35.636	1.00		A
50			0									
	ATOM	2069	N	GLY			45.844	17.133	34.167	1.00	16.23	Α
	MOTA	2070	CA	GLY	Α	332	45.420	16.353	33.015	1.00	14.10	Α
	ATOM	2071	С	GLY			43.982	16.154	32.596	1.00		Α
	ATOM	2072	0	GLY			43.063	16.864	33.017	1.00		Α
55	ATOM	2073	N	TYR	Α	333	43.804	15.141	31.750	1.00	14.37	Α
	MOTA	2074	CA	TYR	Α	333	42.510	14.806	31.182	1.00	13.56	Α
	ATOM	2075	СВ	TYR			42.722	13.892	29.968	1.00		A
	ATOM	2076	CG	TYR			43.153	14.683	28.752	1.00		Α
	MOTA	2077	CD1	TYR	Α	333	42.206	15.172	27.849	1.00	15.29	А

	ATOM	2078	CE1	TYR	A	333	42.573	16.002	26.794	1.00 1	3.42	Α
	ATOM	2079	CD2	TYR	А	333	44.490	15.039	28.561	1.00 1	4.91	Α
	MOTA	2080	CE2	TYR	Α	333	44.872	15.877	27.499	1.00 1	4.87	Α
	MOTA	2081	CZ	TYR	Α	333	43.902	16.353	26.626	1.00 1	5.61	Α
5	MOTA	2082	OH	TYR	Α	333	44.244	17.197	25.599	1.00 1	7.29	Α
	MOTA	2083	С	TYR	Α	333	41.470	14.230	32.127	1.00 1	5.23	Α
	MOTA	2084	0	TYR	Α	333	40.278	14.323	31.846	1.00 1	6.63	Α
	MOTA	2085	N	GLY	Α	334	41.907	13.650	33.244	1.00 1	5.50	Α
	MOTA	2086	CA	GLY	Α	334	40.957	13.100	34.202	1.00 1	5.07	Α
10	ATOM	2087	С	GLY	А	334	39.925	14.146	34.616	1.00 1	6.40	Α
	MOTA	2088	0	GLY	А	334	38.724	13.946	34.433	1.00 1	5.05	Α
	MOTA	2089	N	PRO	Α	335	40.366	15.278	35.184	1.00 1	4.96	Α
	MOTA	2090	CD	PRO	Α	335	41.727	15.531	35.689	1.00 1		Α
	MOTA	2091	CA	PRO	А	335	39.444	16.339	35.606	1.00 1	5.29	А
15	MOTA	2092	СВ	PRO			40.383	17.397	36.178	1.00 1		Α
	MOTA	2093	CG	PRO	А	335	41.485	16.569	36.758	1.00 1	3.81	Α
	ATOM	2094	С	PRO			38.594	16.877	34.448	1.00 1	5.84	Α
	ATOM	2095	0	PRO			37.423	17.204	34.631	1.00 1		Α
	MOTA	2096	N	LEU			39.184	16.971	33.257	1.00 1		А
20	MOTA	2097	CA	LEU			38.450	17.465	32.094	1.00 1		А
	MOTA	2098	СВ	LEU			39.396	17.653	30.898	1.00 1		А
	MOTA	2099	CG	LEU			38.770	17.991	29.538	1.00 1		А
	MOTA	2100		LEU			37.836	19.182	29.662	1.00 1		А
~ -	ATOM	2101		LEU			39.884	18.285	28.528	1.00 1		Α
25	ATOM	2102	С	LEU			37.321	16.508	31.714	1.00 1		Α
	ATOM	2103	0	LEU			36.176	16.921	31.540	1.00 1		Α
	ATOM	2104	N	LYS			37.640	15.225	31.592	1.00 1		A
	ATOM	2105	CA	LYS			36.624	14.243	31.235	1.00 1		A
20	ATOM	2106	СВ	LYS			37.293	12.900	30.921	1.00 1		A
30	ATOM	2107	CG	LYS			38.170	12.994	29.676	1.00 2		A
	ATOM	2108	CD	LYS			39.213	11.892	29.592	1.00 2		A
	ATOM	2109	CE	LYS			38.620	10.560	29.189	1.00 2		A
	ATOM	2110	ΝZ	LYS			39.710	9.560	28.997	1.00 2		A
25	ATOM	2111	C	LYS			35.577	14.096	32.342	1.00 1		A
35	ATOM	2112	O	LYS			34.456	13.652	32.090	1.00 1		A
	ATOM	2113	N	ALA			35.928	14.500	33.559	1.00 1 1.00 1		A
	ATOM ATOM	2114 2115	CA	ALA ALA			34.989 35.749	14.395 14.167	34.674	1.00 1		A
	ATOM	2115	CB C	ALA			34.095	15.621	35.980 34.804	1.00 1		A A
40	ATOM	2117	0	ALA			33.252	15.621	35.695	1.00 1		A
- 10	ATOM	2118	N	HIS			34.262	16.596	33.918	1.00 1		A
	ATOM	2119	CA	HIS			33.438	17.796	34.004	1.00 1		A
	ATOM	2120	CB	HIS			33.865	18.819	32.949	1.00 1		A
	ATOM	2121	CG	HIS			33.163	20.134	33.074	1.00 2		A
45	ATOM	2122		HIS			33.549	21.299	33.649	1.00 1		A
15	ATOM	2123		HIS			31.880	20.340	32.612	1.00 1		A
	ATOM	2124		HIS			31.506	21.576	32.896	1.00 2		A
	ATOM	2125		HIS			32.500	22.179	33.525	1.00 2		A
	ATOM	2126	C	HIS			31.957	17.448	33.845	1.00 1		A
50	ATOM	2127	0	HIS			31.597	16.576	33.061	1.00 1		A
	MOTA	2128	N	PRO			31.079	18.125	34.606	1.00 1		А
	ATOM	2129	CD	PRO			31.424	19.119	35.640	1.00 1		А
	ATOM	2130	CA	PRO			29.630	17.900	34.569	1.00 2		Α
	ATOM	2131	СВ	PRO			29.091	19.058	35.396	1.00 2		A
55	ATOM	2132	CG	PRO			30.146	19.207	36.454	1.00 1		Α
	ATOM	2133	С	PRO			29.000	17.834	33.176	1.00 2		Α
	ATOM	2134	0	PRO			28.049	17.088	32.955	1.00 2		Α
	ATOM	2135	N	PHE			29.528	18.606	32.237	1.00 2		Α
	ATOM	2136	CA	PHE	Α	341	28.985	18.610	30.886	1.00 2		А

	ATOM	2137	СВ	PHE	A	341	29.739	19.624	30.017	1.00 21.6	4 A
	ATOM	2138	CG			341	29.207	19.740	28.613	1.00 23.1	
	ATOM	2139		PHE			27.903	20.171	28.382	1.00 22.5	
	ATOM	2140		PHE			30.013	19.431	27.522	1.00 21.9	
5	ATOM	2141		PHE			27.410	20.292	27.082	1.00 23.5	
	ATOM	2142		PHE			29.533	19.548	26.220	1.00 21.8	
	ATOM	2143	CZ			341	28.228	19.980	25.998	1.00 23.2	
	ATOM	2144	C			341	29.055	17.226	30.237	1.00 21.8	
	ATOM	2145	0			341	28.232	16.896	29.389	1.00 20.3	
10	ATOM	2146	N			342	30.034	16.422	30.640	1.00 20.5	
10	ATOM	2147	CA			342	30.221	15.085	30.077	1.00 23.0	
	ATOM	2148	CB			342	31.710	14.809	29.850	1.00 23.0	
	ATOM	2149	CG			342	32.398	15.812	28.971	1.00 17.0	
	ATOM	2149		PHE			32.010	15.012	27.652	1.00 17.0	
15		2150		PHE			33.487	16.534	29.450	1.00 17.7	
13	ATOM	2151		PHE			32.702	16.867	26.811	1.00 13.7	
	ATOM										
	ATOM	2153		PHE			34.184	17.414	28.617	1.00 17.4	
	ATOM	2154	CZ			342	33.790	17.578	27.298	1.00 16.5	
20	ATOM	2155	C			342	29.679	13.972	30.976	1.00 24.9	
20	ATOM	2156	0			342	30.002	12.798	30.777	1.00 23.9	
	ATOM	2157	N			343	28.861	14.333	31.958	1.00 27.3	
	ATOM	2158 2159	CA			343	28.325	13.349	32.897	1.00 30.2	
	ATOM		CB			343	27.187	13.964	33.716	1.00 32.2	
25	ATOM	2160	CG			343 343	26.581	12.991	34.714	1.00 39.7 1.00 44.7	
23	ATOM	2161	CD	GLU			25.628	13.661	35.688	1.00 44.7	
	ATOM	2162					24.661	14.314	35.234 36.911		
	ATOM	2163 2164		GLU		343	25.847	13.526		1.00 46.8 1.00 28.9	
	ATOM		C				27.852	12.017	32.305		
30	ATOM	2165 2166	O			343 344	28.225	10.952 12.067	32.800 31.258	1.00 31.7 1.00 26.0	
30	ATOM ATOM	2166	N CA			344	27.037 26.520	10.838	30.656	1.00 28.0	
	ATOM	2168	CB			344	25.129	11.089	30.067	1.00 28.7	
	ATOM	2169	OG			344	25.203	11.942	28.940	1.00 28.7	
	ATOM	2170	C			344	27.407	10.214	29.577	1.00 30.9	
35	ATOM	2171	0			344	26.987	9.281	28.900	1.00 27.0	
33	ATOM	2172	N			345	28.627	10.715	29.419	1.00 26.7	
	ATOM	2173	CA			345	29.534	10.713	28.402	1.00 23.4	
	ATOM	2173	CB			345	30.565	11.256	27.950	1.00 23.4	
	ATOM	2175		VAL			31.589	10.631	26.995	1.00 23.1	
40	ATOM	2176		VAL			29.854	12.418	27.275	1.00 20.0	
T U	ATOM	2177	C			345	30.326	8.957	28.855	1.00 24.2	
	ATOM	2178	0			345	30.876	8.930	29.960	1.00 24.2	
	ATOM	2179	N			346	30.374	7.942	27.997	1.00 22.0	
	ATOM	2180	CA			346	31.153	6.740	28.272	1.00 21.7	
45	ATOM	2181	CB			346	30.391	5.455	27.857	1.00 26.5	
7.5	ATOM	2182		THR			29.248	5.284	28.706	1.00 20.9	
	ATOM	2183		THR			31.289	4.231	27.990	1.00 24.2	
	ATOM	2184	C			346	32.383	6.945	27.385	1.00 23.4	
	ATOM	2185	0			346	32.306	6.827	26.160	1.00 24.5	
50	ATOM	2186	N			347	33.508	7.270	28.013	1.00 22.9	
20	ATOM	2187	CA			347	34.744	7.569	27.300	1.00 23.8	
	ATOM	2188	СВ			347	35.683	8.352	28.219	1.00 22.5	
	ATOM	2189	CG			347	35.128	9.658	28.693	1.00 20.6	
	ATOM	2190		TRP			35.257	10.927	28.040	1.00 19.1	
55	ATOM	2191		TRP			34.581	11.881	28.838	1.00 18.3	
22	ATOM	2192		TRP			35.878	11.351	26.858	1.00 18.1	
	ATOM	2193		TRP			34.397	9.883	29.828	1.00 18.3	
	ATOM	2194		TRP			34.065	11.218	29.923	1.00 10.5	
	ATOM	2195		TRP			34.510	13.234	28.491	1.00 16.8	
											

	ATOM	2196	CZ3	TRP A	347	35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197	CH2	TRP A	347	35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	C	TRP A		35.538	6.429	26.675	1.00 25.79	A
	MOTA	2199	0	TRP A		36.304	6.654	25.742	1.00 24.67	A
5	MOTA	2200	N	ALA A	. 348	35.360	5.215	27.183	1.00 27.10	A
	ATOM	2201	CA	ALA A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	СВ	ALA A		35.899	2.869	27.636	1.00 27.09	А
	ATOM	2203	С	ALA A		35.895	3.620	25.256	1.00 27.18	A
	ATOM	2204	0	ALA A		36.830	3.148	24.613	1.00 29.41	A
10	MOTA	2205	N	ASN A	. 349	34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN A	349	34.418	3.310	23.375	1.00 27.28	А
	ATOM	2207	СВ	ASN A	349	33.700	1.962	23.444	1.00 29.37	А
	ATOM	2208	CG	ASN A		32.299	2.088	24.013	1.00 30.92	A
	ATOM	2209		ASN A		32.045	2.942	24.859	1.00 30.17	A
15	ATOM	2210	ND2	ASN A	. 349	31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	С	ASN A	349	33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	0	ASN A	349	32.669	3.843	21.819	1.00 25.87	A
	ATOM	2213	N	LEU A		33.947	5.543	22.518	1.00 24.45	A
• •	ATOM	2214	CA	LEU A		33.203	6.510	21.721	1.00 23.14	A
20	ATOM	2215	СВ	LEU A		33.837	7.898	21.848	1.00 23.22	A
	MOTA	2216	CG	LEU A	. 350	33.659	8.605	23.191	1.00 21.05	A
	MOTA	2217	CD1	LEU A	350	34.646	9.756	23.293	1.00 19.36	A
	ATOM	2218	CD2			32.220	9.094	23.319	1.00 18.78	А
	ATOM	2219	C	LEU A		33.082	6.152	20.240	1.00 22.60	
2.5										A
25	ATOM	2220	0	LEU A		32.011	6.296	19.650	1.00 21.15	A
	MOTA	2221	N	HIS A	. 351	34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS A	351	34.089	5.387	18.204	1.00 27.83	A
	ATOM	2223	СВ	HIS A	351	35.506	5.325	17.596	1.00 29.36	A
	ATOM	2224	CG	HIS A		36.082	3.950	17.493	1.00 32.07	A
20										
30	ATOM	2225		HIS A		36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226		HIS A		36.197	3.285	16.291	1.00 33.02	A
	MOTA	2227	CE1	HIS A	. 351	36.775	2.113	16.493	1.00 33.58	A
	MOTA	2228	NE2	HIS A	351	37.036	1.992	17.782	1.00 31.76	A
	ATOM	2229	С	HIS A	3.5.1	33.258	4.144	17.874	1.00 28.12	A
35	ATOM	2230	0	HIS A		33.015	3.847	16.707	1.00 29.49	A
33										
	ATOM	2231	N	GLN A		32.800	3.442	18.908	1.00 29.28	A
	MOTA	2232	CA	GLN A	. 352	31.963	2.255	18.726	1.00 29.67	A
	MOTA	2233	СВ	GLN	352	32.366	1.145	19.694	0.50 30.56	AC1
	ATOM	2234	CG	GLN	352	33.169	0.041	19.041	0.50 30.88	AC1
40	ATOM	2235	CD	GLN	352	34.493	-0.186	19.729	0.50 31.21	AC1
10	ATOM	2236		GLN	352	34.541	-0.450	20.928	0.50 30.76	AC1
	ATOM	2237	NE2	GLN	352	35.578	-0.084	18.971	0.50 32.30	AC1
	MOTA	2238	С	GLN A	. 352	30.504	2.638	18.963	1.00 30.42	A
	MOTA	2239	0	GLN A	352	29.595	1.831	18.770	1.00 29.01	A
45	ATOM	2240	N	GLN A	353	30.290	3.875	19.397	1.00 27.64	A
	ATOM	2241	CA	GLN A		28.948	4.365	19.652	1.00 27.42	A
	ATOM	2242	СВ	GLN A		28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG	GLN A	. 353	29.408	4.837	22.115	1.00 27.34	A
	MOTA	2244	CD	GLN A	353	29.638	5.914	23.156	1.00 27.19	A
50	ATOM	2245	OE1	GLN A	353	28.875	6.872	23.252	1.00 28.29	А
	ATOM	2246		GLN A		30.687	5.753	23.951	1.00 28.79	А
	ATOM	2247	С	GLN A		28.375	4.989	18.385	1.00 29.00	A
	MOTA	2248	0	GLN A		29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR A	354	27.053	4.984	18.276	1.00 27.31	A
55	ATOM	2250	CA	THR A	354	26.390	5.568	17.119	1.00 27.85	A
	ATOM	2251	СВ	THR A		24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.03	A
	ATOM	2253	CG2			24.289	5.585	15.709	1.00 29.58	A
	ATOM	2254	С	THR A	354	26.244	7.062	17.376	1.00 26.85	A

	ATOM	2255	0	THR	Α	354	25.592	7.475	18.329	1.00 25	.77	Α
	ATOM	2256	N			355	26.867	7.898	16.533	1.00 27	2.2	Α
	MOTA	2257	CD	PRO	Α	355	27.792	7.588	15.431	1.00 25	.89	Α
	ATOM	2258	CA	PRO	Α	355	26.763	9.346	16.734	1.00 27	.23	Α
5	ATOM	2259	СВ	PRO			27.625	9.915	15.609	1.00 24		A
5												
	MOTA	2260	CG	PRO	Α	355	28.643	8.838	15.385	1.00 25	.54	Α
	ATOM	2261	С	PRO	Α	355	25.322	9.837	16.641	1.00 28	.07	Α
	ATOM	2262	0	PR∩	Ζ	355	24.548	9.364	15.810	1.00 27		Α
	ATOM	2263	N			356	24.941	10.792	17.500	1.00 28		Α
10	MOTA	2264	CD	PRO	Α	356	25.752	11.560	18.462	1.00 28	.31	Α
	ATOM	2265	CA	PRO	Α	356	23.572	11.306	17.448	1.00 28	. 44	Α
	ATOM	2266	СВ	DD○	7\	356	23.539	12.301	18.604	1.00 28		Α
	ATOM	2267	CG			356	24.946	12.832	18.612	1.00 26		Α
	MOTA	2268	С	PRO	Α	356	23.363	11.978	16.097	1.00 29	.25	Α
15	ATOM	2269	0	PRO	Α	356	24.304	12.537	15.529	1.00 27	.27	Α
	ATOM	2270	N	ALA			22.143	11.910	15.575	1.00 30		Α
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00 32		Α
	MOTA	2272	СВ	ALA	Α	357	20.507	12.019	13.757	1.00 31	.99	Α
	ATOM	2273	С	ALA	Α	357	21.824	14.035	14.448	1.00 35	.05	Α
20	ATOM	2274	0	ALA			21.194	14.561	15.369	1.00 35		A
20												
	ATOM	2275	N	LEU	А	358	22.516	14.730	13.552	1.00 37		Α
	ATOM	2276	CA	LEU	Α	358	22.578	16.185	13.597	1.00 42	.15	Α
	ATOM	2277	СВ	LEU	Α	358	23.679	16.681	12.658	1.00 39	. 5.4	Α
	ATOM	2278	CG	LEU			25.086	16.285	13.109	1.00 39		
												Α
25	MOTA	2279	CD1	LEU	Α	358	26.102	16.686	12.062	1.00 39	.29	Α
	ATOM	2280	CD2	LEU	Α	358	25.395	16.953	14.445	1.00 40	.01	Α
	ATOM	2281	С	LEU	Δ	358	21.241	16.837	13.242	1.00 45	91	Α
	ATOM	2282	0	LEU			20.874	16.927	12.069	1.00 45		A
	MOTA	2283	N	THR	Α	359	20.530	17.290	14.275	1.00 50	.06	Α
30	ATOM	2284	CA	THR	Α	359	19.223	17.939	14.140	1.00 53	.73	Α
	ATOM	2285	СВ	THR			19.353	19.428	13.726	1.00 54		Α
	ATOM	2286		THR			19.995	19.521	12.448	1.00 56		Α
	MOTA	2287	CG2	THR	Α	359	20.158	20.204	14.763	1.00 54	.32	Α
	ATOM	2288	С	THR	Α	359	18.309	17.236	13.139	1.00 54	.47	Α
35	ATOM	2289	0	THR			18.483	16.016	12.930	1.00 55		A
33												
	ATOM	2290	OXT	THR			17.407	17.908	12.595	1.00 56		Α
	ATOM	2291	OH2	TIP	S	1	42.566	19.118	34.302	1.00 15	.09	S
	ATOM	2292	OH2	TIP	S	2	41.052	32.378	19.857	1.00 15	.82	S
	ATOM	2293	OH2		S	3	37.014	33.030	17.747	1.00 16		S
40												
40	ATOM	2294			S	5	45.353	24.370	18.152	1.00 16		S
	MOTA	2295	OH2	TIP	S	6	31.896	13.930	33.235	1.00 20	.42	S
	ATOM	2296	OH2	TIP	S	7	50.351	22.781	28.249	1.00 21	.14	S
	ATOM	2297		TIP		8	45.246	-0.589	-0.734	1.00 17		S
	ATOM	2298		TIP		11	46.249	-0.348	-8.523	1.00 21		S
45	MOTA	2299	OH2	TIP	S	14	45.756	11.148	29.680	1.00 21	.94	S
	ATOM	2300	OH2	TIP	S	15	44.273	13.157	34.592	1.00 15	. 61	S
								3.722	-1.720			S
	ATOM	2301		TIP		17	53.598			1.00 21		
	ATOM	2302	OH2	TIP	S	18	46.049	13.087	31.565	1.00 20	.35	S
	ATOM	2303	OH2	TIP	S	19	53.422	22.401	-3.280	1.00 23	.26	S
50	ATOM	2304		TIP		20	34.587	7.922	5.383	1.00 22		S
•												
	ATOM	2305		TIP		21	45.053	27.379	19.376	1.00 29		S
	ATOM	2306		TIP		23	28.899	36.416	28.633	1.00 31		S
	MOTA	2307	OH2	TIP	S	24	35.531	11.645	-8.219	1.00 23	.45	S
	ATOM	2308		TIP		25	47.364	28.787	19.612	1.00 23		S
55												
55	ATOM	2309		TIP		27	48.859	21.588	12.634	1.00 23		S
	ATOM	2310	OH2	TIP	S	29	48.805	8.920	23.626	1.00 22	.23	S
	ATOM	2311	OH2	TIP	S	31	48.619	7.247	10.112	1.00 21	.32	S
	ATOM	2312		TIP		34	44.824	28.720	15.621	1.00 25		S
						35						S
	ATOM	2313	OnZ	TIP	S	J J	26.030	12.634	13.407	1.00 21	· 0 T	S

	MOTA	2314	OH2 TI	P S	36	50.462	19.810	40.066	1.00 25.	45	S
	ATOM	2315	OH2 TI	P S	37	39.631	23.510	-0.239	1.00 30.	88	S
	ATOM	2316	OH2 TI			44.734	42.655	10.346	1.00 30.		S
	ATOM	2317	OH2 TI			54.653	3.902	1.503	1.00 27.		S
5	MOTA	2318	OH2 TI	P S	4.5	45.693	21.923	39.754	1.00 28.	30	S
	ATOM	2319	OH2 TI	P S	47	47.820	16.413	7.805	1.00 25.	73	S
	ATOM	2320	OH2 TI			50.292	31.412	29.642	1.00 32.		S
	ATOM	2321	OH2 TI			26.056	16.646	34.827	1.00 29.		S
	ATOM	2322	OH2 TI	P S	52	31.714	10.996	31.855	1.00 29.	15	S
10	ATOM	2323	OH2 TI	P S	53	46.108	23.843	-4.299	1.00 24.	21	S
	ATOM	2324	OH2 TI	P S	54	37.645	11.206	34.448	1.00 28.	56	S
		2325	OH2 TI			26.371	28.513	12.142	1.00 32.		S
	ATOM										
	ATOM	2326	OH2 TI			33.564	19.700	3.483	1.00 28.		S
	ATOM	2327	OH2 TI	P S	64	48.295	-0.632	14.280	1.00 32.	13	S
15	ATOM	2328	OH2 TI	P S	65	40.064	26.036	34.324	1.00 24.	17	S
	ATOM	2329	OH2 TI	P S	66	29.570	3.958	14.729	1.00 28.	94	S
	ATOM	2330	OH2 TI			60.085	11.604	6.814	1.00 38.		S
	ATOM	2331	OH2 TI			39.203	44.403	18.686	1.00 26.		S
	MOTA	2332	OH2 TI	P S	76	47.312	12.366	27.366	1.00 28.	51	S
20	ATOM	2333	OH2 TI	P S	8.0	43.862	33.771	33.329	1.00 28.	82	S
	ATOM	2334	OH2 TI	P S	81	57.890	13.106	2.128	1.00 40.	62	S
	ATOM	2335	OH2 TI			41.663	34.381	32.043	1.00 19.		S
	ATOM	2336	OH2 TI			50.974	40.331	19.200	1.00 21.		S
	ATOM	2337	OH2 TI	P S	8.8	47.925	-0.832	-6.556	1.00 24.	11	S
25	MOTA	2338	OH2 TI	P S	90	27.231	28.336	33.481	1.00 27.	64	S
	ATOM	2339	OH2 TI	P S	91	43.651	-7.101	-7.995	1.00 24.	33	S
	ATOM	2340	OH2 TI			49.325	4.387	19.370	1.00 28.		S
	ATOM	2341		P S		46.231	11.549	33.898	1.00 29.		S
	ATOM	2342	OH2 TI	P S	94	63.889	24.831	1.168	1.00 26.	53	S
30	ATOM	2343	OH2 TI	P S	96	56.396	4.952	-6.749	1.00 28.	00	S
	ATOM	2344	OH2 TI	P S	98	35.510	27.986	11.558	1.00 29.	24	S
	ATOM	2345		P S	100	49.942	24.366	30.265	1.00 31.		S
	ATOM	2346	OH2 TI			56.121	7.113	-8.298	1.00 31.		S
	ATOM	2347	OH2 TI			58.318	19.957	-8.378	1.00 26.		S
35	ATOM	2348	OH2 TI	P S	103	49.647	22.446	39.624	1.00 40.	57	S
	ATOM	2349	OH2 TI	P S	104	45.359	7.052	13.052	1.00 26.	27	S
	ATOM	2350	OH2 TI	P S	105	37.150	32.340	32.346	1.00 34.	4.5	S
	ATOM	2351	OH2 TI			43.465	40.457	8.240	1.00 40.		S
	MOTA	2352		P S		36.644	8.257	13.418	1.00 30.		S
40	ATOM	2353	OH2 TI	P S	123	41.912	-8.974	-8.264	1.00 26.	08	S
	MOTA	2354	OH2 TI	P S	124	62.424	15.800	-7.411	1.00 24.	08	S
	ATOM	2355	OH2 TI	P S	126	37.266	18.656	-9.097	1.00 28.	99	S
	ATOM	2356	OH2 TI			43.129	26.845	14.606	1.00 25.		S
	ATOM	2357	OH2 TI			36.339	32.639	29.802	1.00 29.		S
4.5											
45	ATOM	2358	OH2 TI			54.051	14.561	26.498	1.00 33.		S
	MOTA	2359	OH2 TI	P S	131	41.805	-4.242	5.492	1.00 33.	72	S
	ATOM	2360	OH2 TI	P S	133	38.873	25.163	36.697	1.00 30.	69	S
	ATOM	2361	OH2 TI			28.777	8.553	25.307	1.00 31.		S
	ATOM	2362	OH2 TI			53.672		-12.803	1.00 33.		S
50											
50	ATOM	2363	OH2 TI			59.892	15.434	11.467	1.00 31.		S
	ATOM	2364	OH2 TI	P S	137	31.040	12.361	35.470	1.00 34.	07	S
	ATOM	2365	OH2 TI	P S	139	33.489	14.292	-0.598	1.00 40.	68	S
	ATOM	2366	OH2 TI	P S	140	46.918	8.748	11.662	1.00 29.	23	S
	ATOM	2367	OH2 TI			46.297	-7.287	-9.196	1.00 42.		S
55											
55	ATOM	2368	OH2 TI			58.193	6.715	-4.685	1.00 35.		S
	ATOM	2369	OH2 TI			44.598	4.435	12.503	1.00 27.		S
	MOTA	2370	OH2 TI	P S	144	27.003	5.999	12.450	1.00 36.	30	S
	ATOM	2371	OH2 TI	P S	145	43.676	32.852	35.735	1.00 35.	70	S
	ATOM	2372	OH2 TI			35.783	18.628	36.452	1.00 34.		S
	VI OM	2012	U112 11	r 13	T-10	55.705	10.020	JU.7J4	1.00 34.	U-2	D

	ATOM	2373	OH2 TI	P S	147	25.402	4.058	20.638	1.00	45.03	S
	ATOM	2374	OH2 TI	P S	148	45.839	35.853	33.724	1.00	35.47	S
	ATOM	2375	OH2 TI	P S	149	22.176	18.976	16.752	1.00	31.87	S
	ATOM	2376	OH2 TI	P S	150	43.986	33.179	10.162	1.00	37.70	S
5	ATOM	2377	OH2 TI	P S	151	50.653	20.347	42.428	1.00	35.80	S
	ATOM	2378	OH2 TI	P S	152	47.843	24.314	9.506	1.00	31.05	S
	ATOM	2379	OH2 TI	P S	153	44.693	5.273	-14.175	1.00	29.90	S
	ATOM	2380	OH2 TI	P S	155	26.560	36.851	31.684	1.00	49.29	S
	ATOM	2381	OH2 TI	P S	156	46.867	8.019	-12.951	1.00	29.21	S
10	MOTA	2382	OH2 TI	P S	157	30.432	28.741	12.438	1.00	37.76	S
	MOTA	2383	OH2 TI	P S	158	41.004	20.553	6.423	1.00	39.53	S
	MOTA	2384	OH2 TI	P S	159	49.258	20.069	29.294	1.00	33.97	S
	MOTA	2385	OH2 TI	P S	160	48.082	28.459	16.489	1.00	33.10	S
	ATOM	2386	OH2 TI	P S	161	47.448	18.625	27.683	1.00	34.87	S
15	ATOM	2387	OH2 TI	P S	162	19.687	20.632	23.411	1.00	35.01	S
	MOTA	2388	OH2 TI	P S	163	32.402	-1.266	22.443	1.00	37.26	S
	ATOM	2389	OH2 TI	P S	164	39.475	33.468	33.237	1.00	35.34	S
	ATOM	2390	OH2 TI	P S	165	44.277	18.950	5.162	1.00	45.14	S
	ATOM	2391	OH2 TI	P S	166	34.797	30.523	10.736		47.55	S
20	MOTA	2392	OH2 TI	P S	167	46.541	3.526	-14.949	1.00	26.54	S
	MOTA	2393	OH2 TI	P S	168	36.333	16.371	1.539	1.00	38.68	S
	MOTA	2394	OH2 TI	P S	169	46.761	38.936	27.403	1.00	34.66	S
	MOTA	2395	OH2 TI	P S	170	24.163	13.264	11.375		41.23	S
	ATOM	2396	OH2 TI			48.459	15.018	31.951		38.11	S
25	ATOM	2397	OH2 TI		172	34.261	23.193	40.004		48.96	S
	ATOM	2398	OH2 TI			45.924	-0.026	13.224		39.55	S
	ATOM	2399		P S		41.384	37.389	32.543		40.74	S
	ATOM	2400	OH2 TI	P S		49.394	35.312	27.150	1.00	44.33	S
	ATOM	2401		P S		29.066	29.942	34.359		41.46	S
30	ATOM	2402	OH2 TI		180	49.354	19.467	7.273		34.56	S
	MOTA	2403		P S		25.298	17.029	31.863		47.74	S
	ATOM	2404		P S		37.071	25.027	4.669		43.87	S
	MOTA	2405	OH2 TI			22.581	7.487	18.691		41.75	S
	MOTA	2406		P S		32.269	7.011	-1.891		48.84	S
35	ATOM	2407	OH2 TI			48.234	0.494	6.833		48.16	S
	ATOM	2408		P S		20.008	14.658	19.211		45.27	S
	ATOM	2409	OH2 TI		188	49.341	22.698	42.272		42.20	S
	ATOM	2410	OH2 TI		190	61.292	18.260	-8.097		45.21	S
40	ATOM	2411	OH2 TI			28.152	10.606	2.819		40.38	S
40	ATOM	2412	OH2 TI			25.626	12.619	23.191		34.27	S
	ATOM	2413	OH2 TI		193	59.876	11.603	1.216		46.54	S
	ATOM	2414			194	57.592		-10.646		45.82	S
	ATOM	2415	OH2 TI			31.509	36.649	21.499		38.73	S
15	ATOM	2416	OH2 TI			50.270	-1.543 8.729	-6.136		42.66	S
45	ATOM	2417	OH2 TI			24.467		13.088		42.78	S
	ATOM	2418	OH2 TI			38.098	8.699	25.759		32.80	S
	ATOM	2419	OH2 TI			57.831 23.888		-13.255		45.31 37.12	S
	ATOM	2420	OH2 TI OH2 TI				22.328	30.524		37.12	S S
50	ATOM ATOM	2421 2422	OH2 TI			47.691 38.653	26.068 7.070	37.666 29.307		50.54	s S
50			OH2 TI				27.583			53.50	S
	ATOM ATOM	2423 2424	OH2 TI			44.424 22.258	2.296	2.092 17.948		47.38	S
	ATOM	2425	OH2 TI			19.843	17.943	23.303		30.36	S
			OH2 TI					24.681		31.32	S
55	ATOM ATOM	2426 2427	OH2 TI			27.647 37.953	11.344 7.817	-9.284		45.97	S S
55	ATOM	2427	OH2 TI			33.845	34.040	12.124		38.11	S
	ATOM	2429	OH2 TI			58.484	15.269	13.717		38.26	S
	ATOM	2429	OH2 TI			48.526	40.920	26.583		35.23	S
	ATOM	2430	OH2 TI			52.094	21.184	38.122		29.86	S
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	ATOM	2432	OH2 TIP	S 223	36.889	5.881	3.281	1.00 37.63	S
	ATOM	2433	OH2 TIP	S 224	47.642	-1.401	-10.684	1.00 34.89	S
	ATOM	2434	OH2 TIP		47.284	2.916	19.133	1.00 34.10	S
	MOTA	2435	OH2 TIP	s 227	42.468	4.463	-15.039	1.00 37.98	S
5	ATOM	2436	OH2 TIP	S 228	19.169	22.832	21.831	1.00 41.57	S
-	ATOM	2437	OH2 TIP		57.592	12.689	14.880	1.00 50.22	S
	ATOM	2438	OH2 TIP		27.102	9.176	5.655	1.00 40.57	S
	ATOM	2439	OH2 TIP	s 233	58.618	9.072	-11.925	1.00 50.71	S
	ATOM	2440	OH2 TIP	S 234	22.822	25.342	19.945	1.00 34.93	S
10	ATOM	2441	OH2 TIP		24.831	32.218	28.901	1.00 37.69	S
10									
	ATOM	2442		S 237	20.045	10.774	16.992	1.00 39.57	S
	MOTA	2443	OH2 TIP	S 238	58.019	19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP	S 239	19.490	20.949	26.114	1.00 34.55	S
	ATOM	2445	OH2 TIP		61.187	26.377	7.346	1.00 39.68	S
1.5									
15	ATOM	2446	OH2 TIP		33.680	38.342	19.389	1.00 48.93	S
	ATOM	2447	OH2 TIP	S 242	51.539	31.612	10.881	1.00 55.65	S
	MOTA	2448	OH2 TIP	S 244	25.872	14.431	30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP		37.332	5.849	9.544	1.00 43.81	S
	ATOM	2450	OH2 TIP		39.087	-1.293	-9.655	1.00 42.96	S
20	MOTA	2451	OH2 TIP	s 258	23.938	30.000	30.010	1.00 38.89	S
	MOTA	2452	OH2 TIP	S 259	24.949	29.749	32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP		32.111	17.986	1.918	1.00 48.36	S
	ATOM	2454	OH2 TIP		21.404	12.876	25.603	1.00 57.17	S
	MOTA	2455	OH2 TIP	S 269	35.425	36.767	12.550	1.00 30.70	S
25	MOTA	2456	OH2 TIP	s 270	52.438	25.529	30.131	1.00 44.85	S
	ATOM	2457	OH2 TIP	s 271	53.299	20.156	36.003	1.00 37.15	S
		2458			50.914	6.919	23.723	1.00 43.29	S
	ATOM								
	ATOM	2459	OH2 TIP	S 274	31.578	30.795	11.014	1.00 50.15	S
	MOTA	2460	OH2 TIP	s 275	26.341	7.243	22.447	1.00 39.40	S
30	MOTA	2461	OH2 TIP	s 276	60.392	18.195	10.235	1.00 37.91	S
	ATOM	2462	OH2 TIP		47.355		-10.821	1.00 48.18	S
	ATOM	2463		S 279	41.304		-16.647	1.00 38.12	S
	MOTA	2464	OH2 TIP	S 282	33.299	21.620	37.881	1.00 46.29	S
	MOTA	2465	OH2 TIP	S 283	56.469	26.112	-8.575	1.00 43.71	S
35	ATOM	2466	OH2 TIP	S 287	48.382	26.573	7.246	1.00 41.43	S
55				s 288	56.240		-11.331	1.00 41.79	S
	ATOM	2467							
	MOTA	2468	OH2 TIP	S 290	49.060	14.978	28.166	1.00 37.03	S
	MOTA	2469	OH2 TIP	S 291	37.095	44.270	26.442	1.00 45.08	S
	ATOM	2470	OH2 TIP	S 292	47.814	-0.384	-13.299	1.00 48.60	S
40	ATOM	2471	OH2 TIP		58.081	2.784	-7.841	1.00 41.89	S
T O									
	ATOM	2472	OH2 TIP		36.447	45.321	18.644	1.00 54.91	S
	MOTA	2473	OH2 TIP	S 299	49.029	23.328	1.767	1.00 30.55	S
	MOTA	2474	OH2 TIP	s 301	24.375	13.771	8.634	1.00 48.47	S
	ATOM	2475	OH2 TIP		47.904	36.798	28.653	1.00 35.76	S
45									
43	ATOM	2476	OH2 TIP		51.156	40.821	27.172	1.00 43.59	S
	ATOM	2477	OH2 TIP	S 306	32.943	28.917	35.227	1.00 42.60	S
	MOTA	2478	OH2 TIP	s 307	58.462	28.373	6.251	1.00 46.15	S
	ATOM	2479	OH2 TIP		41.964	30.940	36.712	1.00 48.26	S
	ATOM	2480	OH2 TIP				-3.336	1.00 50.61	S
50					51.176	-1.922			
50	ATOM	2481	OH2 TIP		21.319	36.868	23.805	1.00 36.97	S
	MOTA	2482	OH2 TIP	S1002	48.880	32.620	27.617	1.00 44.40	S
	ATOM	2483	OH2 TIP	S1003	61.880	19.473	11.767	1.00 45.49	S
	ATOM	2484	OH2 TIP		52.770	21.424	26.815	1.00 24.43	S
	ATOM	2485	OH2 TIP		35.373	29.094	36.197	1.00 35.97	S
55	ATOM	2486	OH2 TIP	S1006	40.815	-6.636	4.389	1.00 43.15	S
	ATOM	2487	OH2 TIP	s1007	44.953	1.286	11.272	1.00 49.45	S
	ATOM	2488	OH2 TIP		21.004	16.168	27.009	1.00 48.51	S
	ATOM	2489	OH2 TIP		47.094	41.786	9.243	1.00 50.10	S
	ATOM	2490	OH2 TIP	S1012	32.479	2.978	14.158	1.00 49.47	S

	ATOM	2491	012	GLC	G	1	48.557	11.372	-12.279	1.00	40.72	G
	ATOM	2492	C11	GLC	G	1	48.836	12.133	-11.097	1.00	38.05	G
	ATOM	2493		GLC		1	49.266		-11.476		38.09	G
_	MOTA	2494		GLC		1	49.559		-10.292		33.99	G
5	MOTA	2495		GLC		1	48.150		-12.257		37.32	G
	ATOM	2496	016	GLC	G	1	48.574	15.582	-12.604	1.00	36.74	G
	ATOM	2497	012	GLC	G	2	40.114	-6.634	-6.562	1.00	33.52	G
	ATOM	2498		GLC		2	38.967	-6.592	-7.404		31.05	G
	ATOM	2499		GLC		2	37.712	-6.417	-6.552		31.56	G
10												
10	ATOM	2500		GLC		2	36.554	-6.406	-7.389		30.70	G
	MOTA	2501	C15	GLC	G	2	37.792	-5.109	-5.761	1.00	30.03	G
	ATOM	2502	016	GLC	G	2	36.609	-4.961	-4.975	1.00	29.66	G
	ATOM	2503	012	GLC	G	3	44.030	8.243	-13.470	1.00	37.90	G
	ATOM	2504		GLC		3	43.950		-13.690		38.47	G
15	ATOM	2505		GLC		3	42.747		-14.579		39.52	G
13												
	ATOM	2506		GLC		3	41.551		-13.942		39.39	G
	ATOM	2507	C15	GLC	G	3	42.878	9.280	-15.934	1.00	41.43	G
	ATOM	2508	016	GLC	G	3	41.736	9.613	-16.731	1.00	40.78	G
	ATOM	2509	012	GLC	G	5	40.556	1.005	2.289	1.00	45.25	G
20	ATOM	2510	C11	GLC	G	5	40.966	2.332	1.960	1.00	40.56	G
20	ATOM	2511		GLC		5	40.187	3.327	2.814		40.36	G
	MOTA	2512		GLC		5	38.791	3.169	2.572		40.71	G
	MOTA	2513		GLC		5	40.619	4.751	2.464		40.04	G
	ATOM	2514	016	GLC	G	5	39.885	5.681	3.256	1.00	36.89	G
25	ATOM	2515	012	GLC	G	6	36.951	22.702	40.046	1.00	63.04	G
	ATOM	2516		GLC		6	37.592	21.583	39.422		62.46	G
	ATOM	2517		GLC		6	38.104	21.978	38.030		61.14	G
	MOTA	2518		GLC		6	39.034	23.054	38.168		61.72	G
	ATOM	2519		GLC		6	36.948	22.429	37.126		60.51	G
30	ATOM	2520	016	GLC	G	6	35.992	21.372	36.960	1.00	58.61	G
	ATOM	2521	012	GLC	G	7	37.316	0.281	14.299	1.00	73.45	G
	ATOM	2522	C11	GLC	G	7	37.655	-0.758	15.222	1.00	72.78	G
	ATOM	2523		GLC		7	36.592	-1.856	15.157		72.98	G
				GLC		7						G
2.5	ATOM	2524					35.320	-1.299	15.498		73.88	
35	ATOM	2525		GLC		7	36.924	-2.989	16.134		73.66	G
	ATOM	2526	016	GLC	G	7	36.972	-2.493	17.478	1.00	75.38	G
	ATOM	2527	012	GLC	G	8	51.921	21.898	5.908	1.00	62.51	G
	ATOM	2528	C11	GLC	G	8	52.447	20.871	5.063	1.00	63.42	G
	ATOM	2529	C13	GLC	G	8	51.476	20.597	3.908	1.00	64.28	G
40	ATOM	2530		GLC		8	51.297	21.794	3.150		66.28	Ğ
40		2531		GLC			50.121				64.49	G
	ATOM					8		20.137	4.448			
	MOTA	2532		GLC		8	49.233	19.886	3.357		64.01	G
	MOTA	2533	012	GLC	G	10	36.044	37.499	29.523	1.00	56.89	G
	ATOM	2534	C11	GLC	G	10	35.164	36.645	30.259	1.00	56.97	G
45	ATOM	2535	C13	GLC	G	10	33.849	36.489	29.494	1.00	56.11	G
	ATOM	2536		GLC		10	33.248	37.772	29.308	1.00	56.44	G
	ATOM	2537		GLC		10	32.900	35.580	30.277		55.84	G
	MOTA	2538		GLC		10	31.674	35.442	29.557		55.39	G
	MOTA	2539	03G	ATP	Ν	1	46.280	25.658	5.170	1.00	51.49	N
50	ATOM	2540	PG	ATP	Ν	1	46.464	25.053	3.691	1.00	52.22	N
	ATOM	2541	01G	ATP	N	1	47.406	23.911	3.763	1.00	51.41	N
	ATOM	2542		ATP		1	46.794	26.182	2.784	1.00	52.07	N
	ATOM	2543		ATP		1	44.976	24.513	3.344		51.01	N
	ATOM	2544	PB	ATP		1	44.560	22.969	3.605		50.20	N
55	ATOM	2545		ATP		1	43.083	22.898	3.669		49.41	N
	MOTA	2546	02B	ATP	N	1	45.345	22.474	4.766	1.00	50.34	N
	ATOM	2547	03A	ATP	N	1	45.070	22.231	2.255	1.00	47.77	N
	ATOM	2548	PA	ATP		1	45.075	20.613	2.121		42.84	N
	ATOM	2549		ATP		1	45.547	20.291	0.754		43.81	N
	AIOM	4343	OIA	AIP	ΤΛ	Τ	40.04/	∠∪.∠9I	0.754	T.00	40.0T	1/1

	ATOM	2550	02A	ATP	Ν	1	45.807	20.035	3.270	1.00	45.03	N	
	ATOM	2551		ATP		1	43.516	20.223	2.245		41.73	N	
	ATOM	2552		ATP		1	42.528	20.925	1.489		37.57	N	
	ATOM	2553		ATP		1	41.127	20.329	1.776		39.45	N	
-													
5	ATOM	2554		ATP		1	40.907	19.024	1.279		37.72	N	
	ATOM	2555		ATP		1	40.777	20.321	3.251		38.48	N	
	MOTA	2556		ATP		1	40.360	21.615	3.697		40.42	N	
	MOTA	2557	C2*	ATP	Ν	1	39.608	19.374	3.270	1.00	37.58	N	
	MOTA	2558	02*	ATP	Ν	1	38.410	20.076	2.924	1.00	35.98	N	
10	ATOM	2559	C1*	ATP	Ν	1	39.939	18.346	2.173	1.00	35.55	N	
	ATOM	2560	Ν9	ATP	Ν	1	40.628	17.156	2.747	1.00	31.76	N	
	ATOM	2561	C8	ATP	Ν	1	41.864	17.126	3.274	1.00	30.49	N	
	ATOM	2562	N7	ATP		1	42.143	15.877	3.667		29.75	N	
	ATOM	2563	C5	ATP		1	41.088	15.118	3.390		27.49	N	
15	ATOM	2564	C4	ATP		1	40.125	15.925	2.810		30.02	N	
13	ATOM	2565	N3	ATP		1	38.937	15.329	2.431		27.11	N	
	ATOM	2566	C2	ATP		1	38.679	14.085	2.615		25.62		
												N	
	ATOM	2567	N1	ATP		1	39.597	13.283	3.175		21.76	N	
• •	ATOM	2568	C6	ATP		1	40.800	13.768	3.571		23.90	N	
20	MOTA	2569	И6	ATP		1	41.698	12.964	4.127		21.94	N	
	ATOM	2570	S	SO4	Ι	1	58.680	8.493	-0.639	1.00	56.05	I	
	MOTA	2571	01	SO4	Ι	1	57.956	7.875	0.483	1.00	58.83	I	
	ATOM	2572	02	SO4	I	1	57.886	9.607	-1.188	1.00	57.04	I	
	MOTA	2573	03	SO4	I	1	58.906	7.478	-1.683	1.00	57.47	I	
25	ATOM	2574	04	SO4	I	1	59.976	9.008	-0.156	1.00	57.51	I	
	MOTA	2575	S	SO4	I	2	39.339	4.855	7.057	1.00	84.24	I	
	ATOM	2576	01	SO4	I	2	39.390	6.175	7.711	1.00	85.02	I	
	ATOM	2577	02	SO4		2	40.101	4.897	5.797	1.00	84.75	I	
	ATOM	2578	03	SO4		2	37.936	4.506	6.766		84.94	I	
30	ATOM	2579	04	SO4		2	39.931	3.842	7.954		84.44	Ī	
50	ATOM	2580	S	SO4		3	38.987	-2.256	3.310	1.00	58.58	I	
	ATOM	2581	01	SO4		3	37.734	-1.675	3.827		59.11	I	
		2582	02	SO4		3					59.91	I	
	ATOM						39.460	-1.454	2.172				
25	ATOM	2583	03	SO4		3	38.743	-3.640	2.866		60.97	I	
35	ATOM	2584	04	SO4		3	40.014	-2.260	4.369	1.00	59.58	I	
	ATOM	2585	S	SO4		4	34.397	5.289	30.981		64.34	I	
	ATOM	2586	01	SO4		4	33.627	6.528	30.742		60.43	I	
	MOTA	2587	02	SO4	Ι	4	34.337	4.427	29.782	1.00	60.11	I	
	MOTA	2588	03	SO4		4	33.816	4.572	32.133	1.00	64.39	I	
40	MOTA	2589	04	SO4	Ι	4	35.806	5.626	31.277	1.00	63.55	I	
	MOTA	2590	S	so4	I	5	55.074	-6.984	-3.711	1.00	75.40	I	
	ATOM	2591	01	SO4	I	5	54.657	-7.518	-2.399	1.00	74.66	I	
	ATOM	2592	02	SO4	I	5	54.209	-5.845	-4.065	1.00	74.96	I	
	MOTA	2593	03	so4	I	5	54.950	-8.034	-4.742	1.00	74.22	I	
45	ATOM	2594	04	SO4	I	5	56.477	-6.532	-3.633	1.00	75.15	I	
	ATOM	2595	02	PO4			57.362	24.998	13.149	1.00	66.76	P	
	ATOM	2596	03	PO4			59.399	26.166	13.761		66.89	P	
	ATOM	2597	04			100	57.761	25.606	15.462		67.43	P	
	ATOM	2598	01	PO4			57.264	27.325			65.91	P	
50							57.204						
50	ATOM	2599	P		P	100		26.025			66.69	P	_
	ATOM	2600	CB	GLU		80	50.411		-13.538		23.31	AC	
	ATOM	2601	CG	GLU		80	51.306		-14.362		24.09	AC	
	ATOM	2602	CD	GLU		80	52.180		-13.509		25.31	AC	
	MOTA	2603		GLU		80	52.841		-12.580		22.80	AC	
55	MOTA	2604	OE2	GLU		80	52.212	7.018	-13.774	0.50	28.07	AC	2
	MOTA	2605	СВ	SER		105	37.582	-1.281	-6.192	0.50	21.16	AC	2
	ATOM	2606	OG	SER		105	37.127	-1.871	-4.988	0.50	20.42	AC	2
	ATOM	2607	СВ	ARG		116	59.520	22.977	-7.867	0.50	31.00	AC	
	ATOM	2608	CG	ARG		116	60.312	24.192	-8.323		32.50	AC	

```
60.266 24.349 -9.838 0.50 34.11
                                                                        AC2
    MOTA
          2609 CD ARG
                          116
                                         25.499 -10.290 0.50 36.67
          2610 NE
                                  61.045
                                                                        AC2
    MOTA
                    ARG
                          116
                                         26.766 -10.035 0.50 37.26
                                  60.729
                                                                        AC2
    MOTA
          2611
                CZ
                    ARG
                          116
                                         27.053 -9.331 0.50 38.99
                                                                        AC2
    MOTA
          2612
                NH1 ARG
                          116
                                  59.642
    MOTA
          2613
                NH2 ARG
                          116
                                  61.503
                                          27.746 -10.479 0.50 37.83
                                                                        AC2
    MOTA
          2614
                СВ
                    LEU
                          145
                                  49.693
                                          8.642
                                                  6.631
                                                        0.50 15.29
                                                                        AC2
    MOTA
          2615
                CG
                    LEU
                          145
                                  50.783
                                           8.664
                                                  5.552
                                                        0.50 14.29
                                                                        AC2
    MOTA
          2616
                CD1 LEU
                          145
                                  50.264
                                          9.373
                                                  4.305
                                                        0.50 8.20
                                                                        AC2
    MOTA
          2617
                CD2 LEU
                          145
                                  52.030
                                          9.361
                                                  6.087
                                                        0.50 10.66
                                                                        AC2
    MOTA
          2618
                СВ
                    ARG
                          183
                                  27.455 16.155
                                                 24.989
                                                        0.50 19.21
                                                                        AC2
          2619
                CG
                    ARG
                          183
                                  28.077
                                         15.397
                                                 26.147
                                                        0.50 18.46
                                                                        AC2
    MOTA
    MOTA
          2620
                CD
                    ARG
                          183
                                  27.002
                                         14.945
                                                 27.127
                                                        0.50 19.72
                                                                        AC2
                          183
                                  26.016
                                         14.086
                                                 26.478
                                                        0.50 18.79
    MOTA
          2621
                NE
                    ARG
                                                                        AC2
          2622
                          183
                                  24.703
                                         14.279
                                                 26.539
                                                        0.50 18.52
    MOTA
                CZ
                    ARG
                                                                        AC2
          2623
                          183
                                  24.213
                                         15.305
                                                 27.221
                                                        0.50 15.35
    MOTA
                NH1 ARG
                                                                        AC2
          2624
                          183
                                  23.881
                                         13.445
                                                 25.915
                                                        0.50 17.55
    MOTA
                NH2 ARG
                                                                        AC2
                                  38.479
    MOTA
          2625
                CB SER
                          191
                                         10.847
                                                 23.036 0.50 16.57
                                                                        AC2
    MOTA
          2626 OG SER
                          191
                                  37.418
                                         10.765 23.973 0.50 18.62
                                                                        AC2
    MOTA
          2627
                СВ
                   GLU
                          209
                                  38.645 24.079
                                                 8.551 0.50 22.02
                                                                        AC2
                                  37.769 25.296
20
    MOTA
          2628 CG
                   GLU
                          209
                                                  8.263 0.50 23.40
                                                                        AC2
    ATOM
          2629
                CD GLU
                          209
                                  37.513 26.175
                                                  9.483 0.50 24.27
                                                                        AC2
          2630 OE1 GLU
    MOTA
                          209
                                 37.076 27.328
                                                 9.288 0.50 25.25
                                                                        AC2
                          209
                                 37.737 25.727 10.629 0.50 20.24
    ATOM
          2631 OE2 GLU
                                                                        AC2
    ATOM
          2632 CB GLN
                          247
                                 38.598 32.546 14.790 0.50 18.71
                                                                        AC2
          2633 CG GLN
                          247
                                 38.077 33.665 13.900 0.50 16.95
25
    ATOM
                                                                        AC2
          2634 CD GLN
                          247
                                 38.614 33.598 12.479 0.50 19.13
                                                                        AC2
    ATOM
          2635
                          247
                                 39.763 33.221 12.246 0.50 17.24
                                                                        AC2
    ATOM
                OE1 GLN
                                 37.780 33.979 11.520 0.50 19.88
          2636 NE2 GLN
                          247
                                                                        AC2
    ATOM
          2637 CE LYS
                          315
                                 34.978 25.150 36.369 0.50 20.49
    ATOM
                                                                        AC2
                                 34.183 24.074 37.023 0.50 17.05
30
    ATOM
          2638 NZ LYS
                          315
                                                                        AC2
         2639 CB GLN
                          352
                                 32.365 1.170 19.731 0.50 31.10
    MOTA
                                                                        AC2
                                         0.778 19.683 0.50 32.11
         2640 CG GLN
                          352
                                 33.833
                                                                        AC2
    ATOM
                                         0.027 18.419 0.50 33.04
         2641 CD GLN
                          352
                                 34.190
    ATOM
                                                                        AC2
    ATOM 2642 OE1 GLN
                         352
                                 33.906 0.485 17.314 0.50 34.87
                                                                        AC2
         2643 NE2 GLN 352
                                 34.819 -1.133 18.575 0.50 32.08
35
    ATOM
                                                                        AC2
    END
```

Example 3: Co-ordinates for the PDK1 fragment without alternate side chains.

```
40
    REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free r= 0.2220
                   r= 0.1954 free r= 0.2224
    REMARK final
    REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
    REMARK rweight= 0.0900 (with wa= 1.29263)
    REMARK target= mlf steps= 30
    REMARK sq= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /dd1/david/projects/PDK1 new/CNS/prot.par
    REMARK parameter file 2 : /ddl/david/projects/PDK1 new/CNS/atp.par
    REMARK parameter file 3 : CNS TOPPAR:water rep.param
    REMARK parameter file 4 : CNS TOPPAR:ion.param
```

```
REMARK parameter file 5 : /ddl/david/projects/PDK1 new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
           B11= -2.766 B22= -2.766 B33= 5.532
B12= -0.375 B13= 0.000 B23= 0.000
    REMARK
    REMARK
    REMARK B-factor correction applied to coordinate array B: 0.031
    REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range: 28210 ( 100.0
    용 )
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                               568 (
                                                                       2.0
    용 )
    REMARK number of reflections rejected:
                                                                  0 (
                                                                       0.0
    용 )
20
    REMARK total number of reflections used:
                                                              27642 (
                                                                      98.0
    용 )
    REMARK number of reflections in working set:
                                                              27063 ( 95.9
    용 )
    REMARK number of reflections in test set:
                                                                579 ( 2.1
2.5
    용 )
    CRYST1 123.013 123.013 47.624 90.00 90.00 120.00 P 32 2 1
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE:16-Apr-2002 18:31:12
                                       created by user: david
    REMARK VERSION: 1.0
30
             1 CB PRO A 71
                                 58.912 -7.251
                                                8.216 1.00 67.78
   ATOM
                                                                      Α
             2 CG PRO A 71
                                59.621 -6.941 9.534 1.00 69.16
    MOTA
                                                                       Α
                                59.493 -6.506 5.894 1.00 67.06
             3 C PRO A 71
    ATOM
             4 O PRO A 71
                                59.196 -5.318 5.766 1.00 66.66
    MOTA
             5 N PRO A 71
                                60.984 -6.073 7.833 1.00 67.86
    ATOM
             6 CD PRO A 71
                                60.554 -5.762 9.207 1.00 68.24
35
  ATOM
    ATOM
             7 CA PRO A 71
                                60.040 -7.035 7.217 1.00 67.75
    MOTA
             8 N
                   PRO A 72
                                59.356 -7.385 4.890 1.00 66.32
    MOTA
            9 CD PRO A 72
                                59.712 -8.816 4.898 1.00 67.17
    MOTA
            10 CA PRO A 72
                                58.840 -6.986 3.578 1.00 65.61
   ATOM
           11 CB PRO A 72
                                58.672 -8.321 2.858 1.00 66.47
           12 CG PRO A 72
                                59.796 -9.133 3.419 1.00 67.57
    ATOM
                                                                      Α
                                57.527 -6.208 3.673 1.00 63.94
    ATOM
           13 C
                   PRO A 72
                                                                      Α
    ATOM
           14 0
                   PRO A 72
                                56.710 -6.451 4.561 1.00 64.11
                                                                      Α
           15 N ALA A 73
                                57.341 -5.268 2.753 1.00 61.57
   MOTA
                                                                      Α
           16 CA ALA A 73
                                56.133 -4.454 2.708 1.00 58.74
   MOTA
                                                                      Α
                                56.438 -3.030 3.165 1.00 58.05
    MOTA
           17 CB ALA A 73
                                                                       Α
    ATOM
            18 C
                   ALA A
                         73
                                55.626 -4.448 1.271 1.00 56.78
                                                                      Α
    ATOM
            19 0
                   ALA A
                          73
                                56.347
                                        -4.834 0.349 1.00 56.95
                                                                      Α
            20 N
                   PRO A
    ATOM
                         74
                                54.372 -4.024
                                                 1.057 1.00 54.15
                                                                      Α
            21 CD PRO A
                         74
                                53.335 -3.610
                                                2.018 1.00 53.31
   ATOM
                                                                      Α
            22 CA PRO A
                          74
                                 53.856 -4.003 -0.314 1.00 52.54
    MOTA
                                                                      Α
    ATOM
                   PRO A
                          74
                                 52.474 -3.375 -0.148 1.00 52.86
            23 CB
                                                                      Α
            24 CG PRO A
                         74
                                 52.067
                                        -3.824
                                                1.226 1.00 52.88
    MOTA
                                                                      Α
            25 C
                   PRO A 74
                                 54.772 -3.167 -1.204 1.00 50.08
    MOTA
                                                                      Α
   ATOM
            26 O
                   PRO A 74
                                 55.559 -2.361 -0.708 1.00 49.96
                                                                      Α
            27 N
                   ALA A 75
    ATOM
                                54.680 -3.366 -2.514 1.00 47.58
                                                                      Α
            28 CA ALA A
                                                -3.446 1.00 44.69
                                55.503 -2.602
    MOTA
                          75
                                                                      Α
            29 CB ALA A 75
                                                -4.870 1.00 46.14
                                55.312 -3.121
    MOTA
                   ALA A 75
                                55.100 -1.134 -3.371 1.00 41.55
           30 C
    ATOM
```

	MOTA	31	0	ALA	Α	75	53.947	-0.813	-3.086	1.00 4	1.01	A
	ATOM	32	N	LYS	Α	76	56.053	-0.245	-3.619	1.00 3	8.31	A
	ATOM	33	CA	LYS		76	55.781	1.184	-3.588	1.00 3		A
_	ATOM	34	СВ	LYS		76	57.053	1.957	-3.930	1.00 3		A
5	MOTA	35	CG	LYS	Α	76	57.123	3.356	-3.350	1.00 4		A
	ATOM	36	CD	LYS	Α	76	57.262	3.316	-1.836	1.00 4	0.04	A
	ATOM	37	CE	LYS	Α	76	57.511	4.705	-1.277	1.00 4	2.08	A
	MOTA	38	NZ	LYS		76	57.681	4.695	0.202	1.00 4		A
	ATOM	39	C	LYS		76	54.708	1.467	-4.638	1.00 3		A
10												
10	MOTA	40	0	LYS		76	54.814	1.005	-5.770	1.00 3		A
	MOTA	41	Ν	LYS	Α	77	53.668	2.207	-4.270	1.00 2	8.59	A
	ATOM	42	CA	LYS	Α	77	52.619	2.517	-5.232	1.00 2	5.72	A
	ATOM	43	СВ	LYS	А	77	51.316	2.865	-4.509	1.00 2	6.22	А
	ATOM	44	CG	LYS		77	50.796	1.731	-3.631	1.00 2		A
15	ATOM	45	CD	LYS		77	49.487	2.089	-2.967	1.00 2		
13												A
	ATOM	46	CE	LYS		77	49.136	1.091	-1.870	1.00 2		A
	ATOM	47	NZ	LYS	Α	77	48.998	-0.296	-2.380	1.00 2	7.17	A
	ATOM	48	С	LYS	Α	77	53.053	3.668	-6.137	1.00 2	4.67	A
	ATOM	49	0	LYS	А	77	54.010	4.377	-5.829	1.00 2	1.60	А
20	ATOM	50	N	ARG		78	52.351	3.838	-7.254	1.00 2		A
20												
	ATOM	51	CA	ARG		78	52.662	4.897	-8.211	1.00 2		A
	ATOM	52	СВ	ARG	Α	78	53.574	4.344	-9.318	1.00 2		A
	ATOM	53	CG	ARG	Α	78	53.017	3.139	-10.050	1.00 3	4.78	A
	ATOM	54	CD	ARG	Α	78	54.092	2.465	-10.896	1.00 4	0.96	A
25	ATOM	55	NE	ARG		78	53.560	1.364	-11.700	1.00 4	8 - 93	А
	ATOM	56	CZ	ARG		78	52.985		-11.203	1.00 5		A
	ATOM	57		ARG		78	52.860	0.113	-9.889	1.00 5		A
	ATOM	58	NH2	ARG		78	52.530	-0.672	-12.022	1.00 5		A
	ATOM	59	С	ARG	Α	78	51.382	5.488	-8.803	1.00 2	3.76	A
30	ATOM	60	0	ARG	Α	78	50.311	4.888	-8.706	1.00 2	4.25	A
	ATOM	61	N	PRO	Δ	79	51.475	6.676	-9.428	1.00 2	1.76	A
	ATOM	62	CD	PRO		79	52.691	7.475	-9.668	1.00 2		A
	MOTA	63	CA	PRO		79	50.301		-10.021	1.00 2		A
	ATOM	64	СВ	PRO	A	79	50.910		-10.816	1.00 2		A
35	MOTA	65	CG	PRO	Α	79	52.124	8.831	-10.014	1.00 2	2.12	A
	ATOM	66	С	PRO	Α	79	49.446	6.413	-10.903	1.00 2	2.86	A
	ATOM	67	0	PRO	Α	79	48.213	6.461	-10.842	1.00 2	0.52	A
	MOTA	68	N	GLU		80	50.103		-11.714	1.00 2		A
							49.403		-12.628			
40	ATOM	69	CA	GLU		80				1.00 2		A
40	MOTA	70	СВ	GLU		80	50.393		-13.571	1.00 2		A
	MOTA	71	CG	GLU	Α	80	51.230	2.907	-12.925	1.00 2	8.75	A
	ATOM	72	CD	GLU	Α	80	52.157	2.224	-13.913	1.00 3	1.99	A
	ATOM	73	OE1	GLU	Α	80	53.072	2.897	-14.433	1.00 3	4.34	A
	ATOM	74		GLU		80	51.969		-14.172	1.00 3		А
45	ATOM	75	C	GLU		80	48.556		-11.912	1.00 2		A
45												
	MOTA	76	0	GLU		80	47.692		-12.530	1.00 2		A
	MOTA	77	Ν	ASP	A	81	48.804	3.413	-10.622	1.00 1	.9.97	A
	MOTA	78	CA	ASP	Α	81	48.026	2.423	-9.874	1.00 1	.9.93	A
	ATOM	79	СВ	ASP	Α	81	48.736	2.029	-8.571	1.00 2	1.19	A
50	ATOM	80	CG	ASP		81	50.089	1.380	-8.807	1.00 2		А
50		81		ASP		81		0.554	-9.731	1.00 2		
	ATOM						50.195					A
	MOTA	82		ASP		81	51.043	1.685	-8.058	1.00 2		A
	MOTA	83	С	ASP		81	46.652	2.975	-9.518	1.00 2		A
	ATOM	84	0	ASP	Α	81	45.793	2.246	-9.015	1.00 1	.9.96	A
55	ATOM	85	N	PHE		82	46.445	4.258	-9.804	1.00 1		А
	ATOM	86	CA	PHE		82	45.200	4.934	-9.465	1.00 1		A
		87				82			-8.427			
	ATOM		CB	PHE			45.475	6.027		1.00 1		A
	ATOM	88	CG	PHE		82	46.134	5.531	-7.175	1.00 1		А
	ATOM	89	CD1	PHE	Α	82	45.371	5.136	-6.084	1.00 1	7.19	A

	MOTA	90	CD2	$_{ m PHE}$	Α	82	47.520	5.460	-7.086	1.00 18.99	A
	MOTA	91	CE1	PHE	Α	82	45.977	4.676	-4.918	1.00 17.12	A
	ATOM	92		PHE		82	48.137	5.000	-5.925	1.00 19.64	А
	ATOM	93	CZ	PHE		82	47.361	4.607	-4.838	1.00 18.00	A
-											
5	ATOM	94	С	PHE		82	44.476		-10.621	1.00 20.81	A
	MOTA	95	0	PHE	A	82	45.066	5.933	-11.649	1.00 20.34	A
	MOTA	96	N	LYS	Α	83	43.182	5.792	-10.411	1.00 19.80	A
	ATOM	97	CA	LYS	Α	83	42.321	6.478	-11.353	1.00 21.65	A
	ATOM	98	СВ	LYS		83	41.096		-11.687	1.00 22.02	A
10											
10	ATOM	99	CG	LYS		83	40.062		-12.550	1.00 28.93	A
	ATOM	100	CD	LYS		83	38.974		-12.981	1.00 34.20	A
	MOTA	101	CE	LYS	Α	83	37.909	6.042	-13.824	1.00 38.10	A
	MOTA	102	NZ	LYS	Α	83	37.179	7.086	-13.043	1.00 43.33	A
	ATOM	103	С	LYS	А	83	41.913	7.702	-10.541	1.00 20.74	А
15	ATOM	104	0	LYS		83	41.084		-9.635	1.00 20.98	A
15											
	ATOM	105	N	PHE		84	42.513		-10.835	1.00 19.99	A
	ATOM	106	CA	PHE		8 4	42.188	10.049	-10.083	1.00 18.63	A
	MOTA	107	СВ	PHE	Α	8 4	43.279	11.103	-10.258	1.00 18.95	A
	MOTA	108	CG	PHE	Α	84	44.571	10.741	-9.587	1.00 17.68	A
20	ATOM	109	CD1	PHE	Α	84	45.498	9.926	-10.224	1.00 18.16	А
	ATOM	110		PHE		84	44.843	11.183	-8.299	1.00 19.66	А
	ATOM	111		PHE		84	46.676	9.556	-9.589	1.00 18.09	A
	ATOM	112		PHE		84	46.021	10.816	-7.653	1.00 18.89	A
	ATOM	113	CZ	PHE	Α	8 4	46.936	10.002	-8.301	1.00 17.33	A
25	ATOM	114	С	PHE	Α	84	40.834	10.617	-10.460	1.00 19.69	A
	ATOM	115	0	PHE	Α	84	40.391	10.489	-11.601	1.00 20.72	A
	ATOM	116	N	GLY		85	40.178	11.233	-9.484	1.00 16.80	А
	ATOM	117	CA	GLY		85	38.872	11.810	-9.716	1.00 17.73	A
• •	ATOM	118	С	GLY		85	38.819	13.280	-9.346	1.00 18.75	A
30	ATOM	119	0	GLY		85	39.740	14.043	-9.650	1.00 18.45	A
	ATOM	120	N	LYS	Α	86	37.753	13.673	-8.659	1.00 16.00	A
	ATOM	121	CA	LYS	A	86	37.571	15.064	-8.278	1.00 18.26	A
	ATOM	122	СВ	LYS		86	36.133	15.302	-7.812	1.00 19.00	A
	ATOM	123	CG	LYS		86	35.793	14.660	-6.481	1.00 21.55	A
25											
35	ATOM	124	CD	LYS		86	34.368	14.981	-6.066	1.00 26.48	A
	ATOM	125	CE	LYS		86	33.994	14.239	-4.793	1.00 31.92	A
	ATOM	126	NZ	LYS	Α	86	32.568	14.457	-4.412	1.00 35.36	A
	ATOM	127	С	LYS	Α	86	38.523	15.571	-7.202	1.00 18.57	A
	ATOM	128	0	LYS	A	86	39.045	14.807	-6.385	1.00 16.77	A
40	ATOM	129	N	ILE		87	38.737	16.881	-7.227	1.00 17.88	А
	ATOM	130	CA	ILE		87	39.577	17.554	-6.256	1.00 18.26	A
											_
	ATOM	131	CB	ILE		87	39.994	18.952	-6.772	1.00 19.60	A
	ATOM	132		ILE		87	40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133	CG1	ILE	A	87	40.968	18.786	-7.945	1.00 21.16	A
45	ATOM	134	CD1	ILE	Α	87	41.412	20.087	-8.588	1.00 25.26	A
	ATOM	135	С	ILE	A	87	38.731	17.709	-4.997	1.00 19.67	A
	ATOM	136	0	ILE		87	37.628	18.249	-5.052	1.00 20.41	А
	ATOM	137	N	LEU		88	39.240	17.229	-3.867	1.00 19.15	A
5 0	ATOM	138	CA	LEU		88	38.508	17.324	-2.611	1.00 20.68	A
50	ATOM	139	СВ	LEU	A	88	38.870	16.151	-1.700	1.00 19.97	A
	ATOM	140	CG	LEU	Α	88	38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141	CD1	LEU	Α	88	39.090	13.692	-1.311	1.00 21.41	А
	ATOM	142		LEU		88	37.029	14.622	-2.359	1.00 18.84	А
	ATOM	143	C	LEU		88	38.815	18.632	-1.901	1.00 23.11	A
55											
55	ATOM	144	0	LEU		88	37.999	19.146	-1.139	1.00 25.10	A
	ATOM	145	N	GLY		89	39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY	Α	89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	С	GLY	Α	89	41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0	GLY		89	42.445	20.202	-2.666	1.00 22.19	А
			-			-					

	ATOM	149	N	GLU	Α	90	41.870	22.254	-1.906	1.00 26.22	A
	ATOM	150	CA	GLU	Ζ.	90	43.064	22.924	-2.404	1.00 29.96	А
	ATOM	151	СВ	GLU	А	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	Α	90	42.267	23.038	-4.831	1.00 34.32	A
5	ATOM	153	CD	GLU	Δ	90	41.711	23.930	-5.927	1.00 38.27	A
5											
	ATOM	154		GLU		90	40.590	24.456	-5.764	1.00 40.57	A
	ATOM	155	OE2	GLU	Α	90	42.398	24.110	-6.952	1.00 40.90	A
	ATOM	156	С	GLU	Α	90	43.711	23.768	-1.313	1.00 30.68	A
	ATOM	157	0	GLU		90	43.049	24.574	-0.668	1.00 32.83	А
10											
10	ATOM	158	N	GLY		91	45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	ca	$\operatorname{GL} Y$	Α	91	45.724	24.332	-0.104	1.00 29.40	A
	ATOM	160	С	GLY	А	91	46.795	25.151	-0.798	1.00 29.98	А
	ATOM	161	0	GLY		91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER		92	47.605	25.870	-0.029	1.00 28.30	A
15	ATOM	163	CA	SER	Α	92	48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	СВ	SER	Α	92	49.165	27.717	0.370	1.00 32.43	A
		165	OG	SER		92	49.520	27.099	1.593	1.00 40.94	A
	ATOM										
	ATOM	166	С	SER	Α	92	49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER	Α	92	50.456	26.221	-2.143	1.00 30.46	A
20	ATOM	168	N	PHE	Δ	93	50.087	24.703	-0.536	1.00 27.65	А
20	ATOM	169				93	51.185		-0.995	1.00 26.34	
			CA	PHE				23.855			A
	ATOM	170	СВ	PHE	Α	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Α	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	Δ	93	52.283	25.909	1.392	1.00 29.96	А
25									-0.308		
23	ATOM	173		PHE		93	53.949	25.613		1.00 31.38	А
	ATOM	174	CE1	PHE	Α	93	52.779	27.181	1.665	1.00 32.69	A
	ATOM	175	CE2	PHE	Α	93	54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE		93	53.864	27.670	0.945	1.00 31.81	А
	ATOM	177	С	PHE		93	50.759	22.445	-1.365	1.00 25.39	A
30	ATOM	178	0	PHE	Α	93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER	A	94	49.457	22.235	-1.519	1.00 23.63	A
	ATOM	180	CA	SER		94	48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	СВ	SER	А	94	49.017	20.013	-0.628	1.00 21.42	A
	MOTA	182	OG	SER	Α	94	48.091	20.475	0.340	1.00 21.19	A
35	ATOM	183	С	SER	Α	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	Ō	SER		94	46.795	21.882	-2.173	1.00 18.76	A
	ATOM	185	N	THR		95	47.174	19.832	-3.038	1.00 19.38	A
	ATOM	186	CA	THR	Α	95	45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	СВ	THR	Α	95	45.818	19.818	-5.110	1.00 19.25	A
40	ATOM	188		THR		95	46.196	21.162	-5.434	1.00 22.04	A
T O											
	ATOM	189	CG2			95	44.421	19.549	-5.661	1.00 17.61	A
	ATOM	190	С	THR	Α	95	45.455	18.201	-3.243	1.00 18.61	A
	ATOM	191	0	THR	Α	95	46.212	17.264	-3.524	1.00 17.10	A
	ATOM	192	N	VAL		96	44.295	18.024	-2.623	1.00 16.53	A
4.5											
45	ATOM	193	CA	VAL	А	96	43.845	16.685	-2.266	1.00 16.05	А
	ATOM	194	СВ	VAL	Α	96	43.170	16.672	-0.886	1.00 16.32	A
	ATOM	195	CG1	VAL	Δ	96	42.741	15.249	-0.532	1.00 18.02	A
		196		VAL		96	44.145	17.206		1.00 16.69	
	ATOM								0.168		A
	ATOM	197	С	VAL	Α	96	42.875	16.207	-3.335	1.00 16.42	A
50	ATOM	198	0	VAL	Α	96	41.906	16.892	-3.665	1.00 16.47	A
	ATOM	199	N	VAL	A	97	43.157	15.033	-3.888	1.00 16.80	А
	ATOM					97	42.338				
		200	CA	VAL				14.471	-4.949	1.00 16.72	A
	ATOM	201	СВ	VAL		97	43.153	14.354	-6.255	1.00 18.43	A
	ATOM	202	CG1	VAL	Α	97	42.249	13.927	-7.404	1.00 19.69	A
55	ATOM	203		VAL		97	43.831	15.685	-6.569	1.00 17.84	А
	ATOM	204	С	VAL		97	41.812	13.091	-4.583	1.00 16.77	A
	ATOM	205	0	VAL		97	42.532	12.270	-4.014	1.00 17.13	A
	ATOM	206	N	LEU	Α	98	40.545	12.845	-4.895	1.00 16.62	A
	ATOM	207	CA	LEU		98	39.947	11.548	-4.624	1.00 17.04	А
		_ 0 /	J2 1					010		1,.01	11

	ATOM	208	CB	LEU	Α	98	38.424	11.633	-4.743	1.00	16.89	A
	ATOM	209	CG	LEU	Ζ	98	37.635	10.342	-4.508	1 00	19.46	А
	MOTA	210		LEU		98	37.990	9.762	-3.146		20.07	A
	ATOM	211	CD2	LEU	Α	98	36.143	10.627	-4.588	1.00	17.93	A
5	ATOM	212	С	LEU	Δ	98	40.512	10.597	-5.677	1.00	17.38	A
,											18.60	
	ATOM	213	0	LEU		98	40.527	10.920	-6.863			A
	ATOM	214	N	ALA	Α	99	40.995	9.438	-5.246	1.00	17.13	A
	ATOM	215	CA	ALA	Α	99	41.570	8.466	-6.168	1.00	18.42	A
	ATOM	216	СВ	ALA	Ζ\	99	43.090	8.524	-6.105	1 00	14.76	А
1.0												
10	ATOM	217	С	ALA		99	41.102	7.055	-5.848		21.40	A
	ATOM	218	0	ALA	Α	99	40.941	6.691	-4.679	1.00	22.52	A
	ATOM	219	N	ARG	Α	100	40.878	6.261	-6.888	1.00	19.77	A
	ATOM	220	CA	ARG			40.459	4.884	-6.693		20.85	A
	MOTA	221	СВ	ARG	А	100	39.202	4.585	-7.518	1.00	24.22	A
15	ATOM	222	CG	ARG	Α	100	38.608	3.205	-7.256	1.00	31.78	A
	ATOM	223	CD	ARG	Α	100	37.326	2.979	-8.048	1.00	36.24	A
		224		ARG			36.213	3.818	-7.594		41.40	
	ATOM		NE									A
	ATOM	225	CZ	ARG	Α	100	35.566	3.662	-6.439	1.00	42.05	A
	ATOM	226	NH1	ARG	Α	100	35.912	2.696	-5.598	1.00	40.67	А
20	ATOM	227	NH2	ARG	Δ	100	34.559	4.468	-6.128	1.00	43.65	А
20												
	ATOM	228	С	ARG			41.613	3.985	-7.129		18.63	A
	ATOM	229	0	ARG	Α	100	42.078	4.065	-8.271	1.00	19.49	A
	ATOM	230	N	GLU	Α	101	42.102	3.157	-6.212	1.00	16.43	А
	ATOM	231	CA	GLU			43.196	2.246	-6.533		16.11	А
25												
25	ATOM	232	СВ	GLU			43.774	1.637	-5.248		16.79	A
	ATOM	233	CG	GLU	Α	101	44.917	0.657	-5.488	1.00	16.51	A
	ATOM	234	CD	GLU	Α	101	45.501	0.115	-4.200	1.00	18.20	A
	ATOM	235		GLU			44.733	-0.081	-3.239		18.32	A
	ATOM	236	OE2	GLU	Α	101	46.725	-0.132	-4.150	1.00	17.14	A
30	ATOM	237	С	GLU	Α	101	42.625	1.152	-7.442	1.00	17.92	A
	ATOM	238	0	GLU	Δ	101	41.681	0.462	-7.069	1.00	18.02	A
		239		LEU			43.198	1.002	-8.632		19.06	
	ATOM		N									A
	ATOM	240	CA	LEU	Α	102	42.718	0.025	-9.607	1.00	20.71	A
	ATOM	241	СВ	LEU	Α	102	43.569	0.097	-10.878	1.00	23.42	A
35	ATOM	242	CG	LEU	Δ	102	43.531	1 426	-11.642	1 00	25.30	A
55									-12.748		27.88	
	ATOM	243		LEU			44.577					A
	ATOM	244	CD2	LEU	Α	102	42.140	1.647	-12.214	1.00	26.79	A
	ATOM	245	С	LEU	Α	102	42.671	-1.418	-9.125	1.00	21.62	A
	ATOM	246	0	LEU	Δ	102	41.668	-2.103	-9.305	1 00	21.09	A
40				ALA								
40	ATOM	247	N				43.753	-1.874	-8.507		19.38	A
	ATOM	248	CA	ALA	Α	103	43.836	-3.249	-8.035	1.00	20.87	A
	ATOM	249	СВ	ALA	Α	103	45.284	-3.571	-7.671	1.00	19.23	A
	ATOM	250	С	ALA			42.919	-3.629	-6.872		19.92	A
									-6.628		20.38	
	ATOM	251	0	ALA			42.703	-4.815				A
45	ATOM	252	N	THR	Α	104	42.361	-2.643	-6.175	1.00	18.12	A
	ATOM	253	CA	THR	Α	104	41.517	-2.927	-5.018	1.00	17.15	A
	ATOM	254	СВ	THR			42.212	-2.484	-3.717		19.54	A
	ATOM	255		THR			42.456	-1.070	-3.773		19.26	A
	ATOM	256	CG2	THR	Α	104	43.536	-3.219	-3.529	1.00	17.02	A
50	ATOM	257	С	THR	Α	104	40.159	-2.247	-5.026	1.00	19.44	A
		258									18.70	
	ATOM		0	THR			39.259	-2.648	-4.285			A
	ATOM	259	N	SER			40.034	-1.207	-5.847		19.65	A
	ATOM	260	CA	SER	Α	105	38.819	-0.400	-5.967	1.00	19.37	A
	ATOM	261	СВ	SER			37.598	-1.304	-6.173		21.81	А
55												
55	ATOM	262	OG	SER			36.431	-0.539	-6.412		23.01	A
	MOTA	263	С	SER	Α	105	38.644	0.447	-4.701	1.00	18.99	A
	ATOM	264	0	SER	Α	105	37.602	1.070	-4.488	1.00	18.66	A
	ATOM	265	N	ARG			39.674	0.468	-3.861		16.84	A
	ATOM	266	CA	ARG	Α	ТΩР	39.655	1.267	-2.634	T.00	16.21	A

					4				4 00 40 11	
	ATOM	267	СВ	ARG A	. 106	40.827	0.886	-1.723	1.00 16.41	A
	ATOM	268	CG	ARG A	. 106	40.619	-0.367	-0.906	1.00 15.49	A
	ATOM	269	CD	ARG A	106	41.887	-0.755	-0.170	1.00 17.43	A
							-1.792	0.824	1.00 20.47	
_	ATOM	270	NE	ARG A		41.620				A
5	ATOM	271	CZ	ARG A	. 106	42.548	-2.568	1.371	1.00 20.24	A
	ATOM	272	NH1	ARG A	. 106	43.821	-2.433	1.017	1.00 17.80	A
	ATOM	273	NH2	ARG A	106	42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG A		39.785	2.746	-2.981	1.00 17.37	A
		275							1.00 17.75	
1.0	ATOM		0	ARG A		40.514	3.103	-3.902		A
10	ATOM	276	N	GLU A	. 107	39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU A	. 107	39.156	5.039	-2.461	1.00 20.80	A
	ATOM	278	СВ	GLU A	. 107	37.779	5.694	-2.337	1.00 22.93	A
	ATOM	279	CG	GLU A	107	36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	GLU A		35.431	5.975	-3.148	1.00 32.40	A
1.5										
15	ATOM	281		GLU A		35.262	6.939	-3.923	1.00 33.74	A
	ATOM	282	OE2	GLU A		34.608	5.654	-2.263	1.00 36.00	A
	ATOM	283	С	GLU A	. 107	40.053	5.678	-1.410	1.00 18.93	A
	ATOM	284	0	GLU A	. 107	39.891	5.427	-0.220	1.00 19.21	A
	ATOM	285	N	TYR A		40.988	6.507	-1.852	1.00 16.70	А
20	ATOM	286	CA	TYR A		41.883	7.209	-0.942	1.00 15.86	A
20										
	ATOM	287	СВ	TYR A		43.325	6.728	-1.104	1.00 15.30	A
	ATOM	288	CG	TYR A	. 108	43.593	5.328	-0.612	1.00 16.33	A
	ATOM	289	CD1	TYR A	. 108	43.765	5.066	0.746	1.00 16.36	A
	ATOM	290	CE1	TYR A	108	44.046	3.769	1.201	1.00 18.48	A
25	ATOM	291		TYR A		43.701	4.268	-1.511	1.00 13.25	A
23	ATOM	292		TYR A		43.980	2.981	-1.075	1.00 17.28	A
	ATOM	293	CZ	TYR A		44.152	2.736	0.276	1.00 19.17	A
	ATOM	294	OH	TYR A	. 108	44.440	1.461	0.688	1.00 19.38	A
	ATOM	295	С	TYR A	. 108	41.850	8.687	-1.292	1.00 16.80	A
30	ATOM	296	0	TYR A	108	41.560	9.058	-2.431	1.00 15.22	A
	ATOM	297	N	ALA A		42.132	9.528	-0.306	1.00 14.61	A
		298				42.207		-0.539	1.00 14.30	
	ATOM		CA	ALA A			10.957			A
	ATOM	299	СВ	ALA A		41.671	11.726	0.661	1.00 14.78	A
	ATOM	300	С	ALA A	. 109	43.713	11.136	-0.667	1.00 16.79	A
35	ATOM	301	0	ALA A	. 109	44.450	10.983	0.317	1.00 16.52	A
	ATOM	302	N	ILE A	. 110	44.182	11.410	-1.881	1.00 14.80	A
	ATOM	303	CA	ILE A		45.609	11.574	-2.093	1.00 15.80	A
	ATOM	304	CB	ILE A		46.065	10.863	-3.396	1.00 16.85	A
4.0	ATOM	305		ILE A		47.550	11.098	-3.632	1.00 16.80	A
40	ATOM	306		ILE A		45.774	9.358	-3.284	1.00 17.76	A
	ATOM	307	CD1	ILE A	. 110	46.308	8.513	-4.437	1.00 16.07	A
	ATOM	308	С	ILE A	. 110	46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE A	110	45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS A		46.846	13.435	-1.177	1.00 16.15	A
15										
45	ATOM	311	CA	LYS A		47.326	14.808	-1.100	1.00 17.20	A
	ATOM	312	СВ	LYS A		47.700	15.176	0.344	1.00 17.41	A
	MOTA	313	CG	LYS A	. 111	48.350	16.547	0.464	1.00 20.71	A
	ATOM	314	CD	LYS A	. 111	48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE	LYS A		47.288	17.381	2.598	1.00 29.46	А
50	ATOM	316	NZ	LYS A		47.516	17.866	4.000	1.00 30.50	A
50										
	ATOM	317	С	LYS A		48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	0	LYS A	. 111	49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N	ILE A	. 112	48.509	15.798	-2.963	1.00 15.87	A
	ATOM	320	CA	ILE A		49.606	15.967	-3.907	1.00 17.28	А
55	ATOM	321	СВ	ILE A		49.079	15.911	-5.358	1.00 16.43	A
55										
	ATOM	322		ILE A		50.235	15.998	-6.341	1.00 15.12	A
	ATOM	323		ILE A		48.293	14.609	-5.565	1.00 16.82	A
	ATOM	324	CD1	ILE A	. 112	47.580	14.511	-6.904	1.00 18.47	A
	ATOM	325	С	ILE A	. 112	50.307	17.301	-3.663	1.00 19.03	A

	ATOM	326	0	ILE A 1	12	49.669	18.350	-3.635	1.00 19.1	5 A
	ATOM	327	N	LEU A 1	1 2	51.622	17.245	-3.472	1.00 20.2	
	MOTA	328	CA	LEU A 1	13	52.416	18.442	-3.214	1.00 22.3	6 A
	ATOM	329	СВ	LEU A 1	13	52.995	18.397	-1.794	1.00 22.1	3 A
_										
5	MOTA	330	CG	LEU A 1		52.042	18.063	-0.646	1.00 22.4	
	ATOM	331	CD1	LEU A 1	13	51.866	16.557	-0.553	1.00 23.8	1 A
	ATOM	332		LEU A 1		52.603	18.595	0.660	1.00 23.6	
	MOTA	333	С	LEU A 1	.13	53.560	18.547	-4.215	1.00 23.3	7 A
	ATOM	334	0	LEU A 1	13	54.300	17.586	-4.424	1.00 23.1	1 A
10	ATOM	335	N	GLU A 1		53.706	19.714	-4.834	1.00 23.8	
10										
	MOTA	336	CA	GLU A 1	14	54.771	19.920	-5.806	1.00 26.0	0 A
	ATOM	337	СВ	GLU A 1	14	54.435	21.111	-6.706	1.00 27.7	4 A
	MOTA	338	CG	GLU A 1		55.533	21.452	-7.696	1.00 35.0	
	MOTA	339	CD	GLU A 1	14	55.220	22.696	-8.497	1.00 39.2	4 A
15	ATOM	340	OE 1	GLU A 1	14	54.808	23.703	-7.885	1.00 41.4	5 A
15										
	ATOM	341	OEZ	GLU A 1	14	55.395	22.670	-9.736	1.00 44.0	5 A
	ATOM	342	С	GLU A 1	14	56.087	20.163	-5.067	1.00 24.3	7 A
	ATOM	343	0	GLU A 1	1 /	56.186	21.071	-4.238	1.00 24.4	3 A
	ATOM	344	N	LYS A 1	.15	57.096	19.350	-5.360	1.00 24.1	0 A
20	ATOM	345	CA	LYS A 1	15	58.376	19.493	-4.678	1.00 24.9	3 A
		346				59.339				
	ATOM		СВ	LYS A 1			18.373	-5.103	1.00 23.7	
	ATOM	347	CG	LYS A 1	15	59.139	17.080	-4.308	1.00 23.0	9 A
	ATOM	348	CD	LYS A 1	1.5	60.064	15.944	-4.743	1.00 21.9	2 A
	ATOM	349	CE	LYS A 1		59.691	15.400	-6.117	1.00 22.4	
25	ATOM	350	NZ	LYS A 1	15	60.447	14.150	-6.448	1.00 19.7	1 A
	ATOM	351	С	LYS A 1	15	59.031	20.858	-4.868	1.00 26.8	7 A
	ATOM	352	0	LYS A 1		59.492	21.469	-3.903	1.00 26.1	
	ATOM	353	N	ARG A 1	16	59.058	21.348	-6.102	1.00 28.7	3 A
	ATOM	354	CA	ARG A 1		59.678	22.638	-6.380	1.00 29.6	
20										
30	ATOM	355	СВ	ARG A 1	16	59.533	22.980	-7.868	1.00 31.2	9 A
	ATOM	356	CG	ARG A 1	16	60.047	24.361	-8.267	1.00 33.1	9 A
	ATOM	357	CD	ARG A 1		61.368	24.710	-7.590	1.00 35.1	
	MOTA	358	NE	ARG A 1	16	62.329	23.612	-7.618	1.00 36.4	2 A
	MOTA	359	CZ	ARG A 1	16	63.510	23.648	-7.009	1.00 36.1	8 A
35		360		ARG A 1		63.871	24.729	-6.332	1.00 36.1	
33	ATOM									
	MOTA	361	NH2	ARG A 1	16	64.324	22.602	-7.067	1.00 35.7	7 A
	ATOM	362	С	ARG A 1	16	59.097	23.761	-5.519	1.00 29.7	0 A
	MOTA	363	0	ARG A 1		59.843	24.515	-4.889	1.00 29.1	
	MOTA	364	N	HIS A 1	17	57.773	23.862	-5.472	1.00 27.2	2 A
40	ATOM	365	CA	HIS A 1	17	57.126	24.903	-4.681	1.00 26.3	3 A
		366	СВ	HIS A 1		55.606	24.835	-4.848	1.00 28.4	
	ATOM									
	MOTA	367	CG	HIS A 1	.17	54.881	26.005	-4.258	1.00 31.8	2 A
	ATOM	368	CD2	HIS A 1	17	55.309	27.249	-3.935	1.00 33.1	9 A
						53.536	25.974			
	MOTA	369		HIS A 1				-3.961	1.00 34.3	
45	MOTA	370	CE1	HIS A 1	17	53.165	27.148	-3.480	1.00 34.5	8 A
	ATOM	371	NE2	HIS A 1	17	54.222	27.940	-3.455	1.00 35.1	8 A
	MOTA	372	С	HIS A 1		57.477	24.780	-3.202	1.00 26.2	
	ATOM	373	0	HIS A 1	17	57.737	25.776	-2.534	1.00 25.6	7 A
	ATOM	374	N	ILE A 1	1.8	57.469	23.554	-2.689	1.00 24.9	
50										
50	MOTA	375	CA	ILE A 1	T8	57.792	23.315	-1.285	1.00 23.9	4 A
	MOTA	376	CB	ILE A 1	18	57.711	21.812	-0.952	1.00 23.5	0 A
	ATOM	377		ILE A 1		58.374	21.533	0.389	1.00 23.7	
	MOTA	378	CG1	ILE A 1	18	56.246	21.362	-0.959	1.00 24.4	2 A
	ATOM	379	CD1	ILE A 1	18	56.066	19.858	-0.834	1.00 28.0	6 A
55										
55	ATOM	380	С	ILE A 1		59.195	23.821	-0.958	1.00 23.7	
	MOTA	381	0	ILE A 1	18	59.402	24.495	0.048	1.00 23.4	9 A
	ATOM	382	N	ILE A 1		60.153	23.489	-1.815	1.00 23.4	
	ATOM	383	CA	ILE A 1		61.534	23.913	-1.619	1.00 25.1	
	ATOM	384	СВ	ILE A 1	19	62.467	23.250	-2.664	1.00 24.2	5 A

	ATOM	385	CG2	ILE A	119	63.858	23.890	-2.617	1.00 22.47	A
	ATOM	386	CG1	ILE A	119	62.540	21.738	-2.395	1.00 25.05	A
	MOTA	387		ILE A		63.327	20.945	-3.439	1.00 24.62	A
	MOTA	388	С	ILE A	119	61.667	25.435	-1.705	1.00 25.96	A
5	ATOM	389	0	ILE A	119	62.330	26.051	-0.872	1.00 24.78	A
	ATOM	390	N	LYS A		61.028	26.039	-2.704	1.00 27.67	A
	MOTA	391	CA	LYS A		61.100	27.489	-2.879	1.00 30.29	A
	MOTA	392	CB	LYS A	120	60.242	27.940	-4.060	1.00 32.34	A
	ATOM	393	CG	LYS A	120	60.674	27.407	-5.409	1.00 39.30	А
10	ATOM	394	CD	LYS A		59.765	27.950	-6.512	1.00 45.19	А
10										
	MOTA	395	CE	LYS A		58.294	27.636	-6.218	1.00 46.48	A
	MOTA	396	NZ	LYS A	120	57.363	28.155	-7.252	1.00 46.49	A
	ATOM	397	С	LYS A	120	60.647	28.247	-1.638	1.00 30.89	A
	ATOM	398	0	LYS A	120	61.303	29.198	-1.217	1.00 32.48	А
1.5										
15	ATOM	399	N	GLU A		59.527	27.825	-1.055	1.00 29.82	A
	ATOM	400	CA	GLU A	121	58.986	28.488	0.128	1.00 30.33	A
	ATOM	401	СВ	GLU A	121	57.455	28.416	0.117	1.00 33.04	A
	ATOM	402	CG	GLU A	121	56.794	29.021	-1.120	1.00 36.45	A
		403	CD	GLU A		57.221	30.456	-1.373	1.00 39.88	
20	ATOM									A
20	MOTA	404		GLU A		57.200	31.264	-0.420	1.00 40.53	A
	MOTA	405	OE2	GLU A	121	57.573	30.778	-2.529	1.00 43.24	A
	ATOM	406	С	GLU A	121	59.511	27.930	1.451	1.00 30.37	A
	ATOM	407	0	GLU A		58.946	28.204	2.513	1.00 31.24	A
	ATOM	408	N	ASN A		60.588	27.151	1.390	1.00 29.03	A
25	ATOM	409	CA	ASN A	122	61.183	26.573	2.594	1.00 28.46	A
	ATOM	410	СВ	ASN A	122	61.836	27.673	3.436	1.00 31.28	A
	ATOM	411	CG	ASN A	122	62.945	28.395	2.698	1.00 34.12	А
	ATOM	412		ASN A		62.697	29.143	1.754	1.00 35.57	A
	MOTA	413	ND2	ASN A		64.181	28.169	3.127	1.00 35.73	A
30	MOTA	414	С	ASN A	122	60.157	25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN A	122	60.085	26.055	4.663	1.00 27.23	A
	ATOM	416	N	LYS A		59.375	24.955	2.842	1.00 23.99	А
	ATOM	417	CA	LYS A		58.358	24.210	3.574	1.00 22.43	A
	MOTA	418	СВ	LYS A	123	57.031	24.248	2.810	1.00 21.97	A
35	ATOM	419	CG	LYS A	123	56.475	25.645	2.599	1.00 25.68	A
	ATOM	420	CD	LYS A	123	56.253	26.354	3.927	1.00 27.54	A
	ATOM	421	CE	LYS A		55.822	27.796	3.716	1.00 31.30	A
	MOTA	422	NZ	LYS A		55.756	28.540	5.004	1.00 33.21	A
	MOTA	423	С	LYS A	123	58.748	22.759	3.821	1.00 22.20	A
40	ATOM	424	0	LYS A	123	57.924	21.960	4.264	1.00 22.50	A
	ATOM	425	N	VAL A	124	59.997	22.412	3.535	1.00 20.59	А
				VAL A						
	ATOM	426	CA			60.439	21.039	3.730	1.00 20.25	A -
	MOTA	427	СВ	VAL A		61.922	20.850	3.328	1.00 19.43	A
	ATOM	428	CG1	VAL A	124	62.346	19.407	3.573	1.00 18.69	A
45	ATOM	429	CG2	VAL A	124	62.104	21.195	1.853	1.00 18.21	A
	ATOM	430	С	VAL A		60.236	20.561	5.163	1.00 19.53	А
	MOTA	431	0	VAL A		59.841	19.418	5.385	1.00 20.02	A
	MOTA	432	N	PRO A	125	60.513	21.422	6.159	1.00 20.01	A
	ATOM	433	CD	PRO A	125	61.178	22.738	6.118	1.00 18.69	A
50	ATOM	434	CA	PRO A		60.318	20.979	7.544	1.00 19.88	А
	ATOM	435	CB	PRO A		60.793	22.180	8.363	1.00 19.95	
										A
	MOTA	436	CG	PRO A		61.839	22.805	7.479	1.00 18.85	A
	MOTA	437	С	PRO A	125	58.848	20.642	7.824	1.00 19.76	A
	ATOM	438	0	PRO A		58.544	19.700	8.550	1.00 16.99	А
55	ATOM	439	N	TYR A		57.947	21.418	7.235	1.00 18.98	A
55										
	ATOM	440	CA	TYR A		56.516	21.220	7.435	1.00 21.97	A
	ATOM	441	CB	TYR A	126	55.752	22.448	6.933	1.00 25.17	A
	ATOM	442	CG	TYR A	126	56.040	23.690	7.748	1.00 30.98	A
	ATOM	443		TYR A		55.438	23.886	8.991	1.00 33.95	А
	7 1 T O I.I	110	011	T T T \ T		33.430	23.000	0.001	1.00 33.33	А

	ATOM	444	CE1	TYR .	A 126	55.72	25.015	9.763	1.00 36.60	A
	ATOM	445	CD2	TYR .	126	56.93	8 24.657	7.292	1.00 35.43	A
	ATOM	446		TYR .		57.23		8.058	1.00 37.20	
	MOTA	447	CZ		A 126	56.61		9.291	1.00 37.40	
5	ATOM	448	OH	TYR .	A 126	56.90	27.073	10.052	1.00 40.85	i A
	ATOM	449	С	TYR .	A 126	55.99	0 19.956	6.762	1.00 21.35	A
	ATOM	450	0	TYR .	A 126	55.26	55 19.175	7.383	1.00 20.49	A
	ATOM	451	N		A 127	56.35		5.501	1.00 18.16	
									1.00 17.58	
1.0	MOTA	452	CA		A 127	55.89		4.790		
10	ATOM	453	СВ		A 127	56.30		3.308	1.00 17.45	
	MOTA	454	CG1	VAL .	A 127	55.78	16 17.350	2.600	1.00 17.97	A
	ATOM	455	CG2	VAL .	A 127	55.75	19.850	2.641	1.00 14.90	A
	ATOM	456	С	VAL .	A 127	56.45	9 17.306	5.448	1.00 18.39	A
	ATOM	457	0	√. Τ.	A 127	55.76		5.583	1.00 18.14	
15	ATOM	458	N		A 128	57.71		5.869	1.00 17.50	
13										
	ATOM	459	CA		A 128	58.37		6.530	1.00 18.54	
	ATOM	460	СВ	THR .	A 128	59.86	16.586	6.805	1.00 18.01	. А
	MOTA	461	og1	THR .	A 128	60.53	7 16.804	5.559	1.00 21.14	A
	ATOM	462	CG2	THR .	A 128	60.53	6 15.446	7.545	1.00 17.95	A
20	ATOM	463	С	THR	A 128	57.67	6 15.941	7.856	1.00 19.49	A
	ATOM	464	0		A 128	57.43		8.179	1.00 18.76	
	ATOM	465	N		A 129	57.34		8.619	1.00 19.60	
	ATOM	466	CA		A 129	56.67		9.904	1.00 20.12	
	ATOM	467	СВ	ARG .	A 129	56.53	18.144	10.621	1.00 21.33	A
25	ATOM	468	CG	ARG .	A 129	55.94	8 18.029	12.023	1.00 28.02	A
	ATOM	469	CD	ARG .	A 129	55.72	19.404	12.597	1.00 31.25	A
	ATOM	470	NE		A 129	56.94		12.560	1.00 37.78	
			CZ		A 129				1.00 40.10	
	ATOM	471				56.96		12.391		
	ATOM	472		ARG .		55.82		12.239	1.00 40.03	
30	ATOM	473	NH2	ARG .	A 129	58.11	.9 22.170	12.374	1.00 44.58	A
	MOTA	474	С	ARG .	A 129	55.28	8 16.186	9.729	1.00 20.08	A
	ATOM	475	0	ARG .	A 129	54.89	15.305	10.496	1.00 20.40	A
	ATOM	476	N		A 130	54.55		8.724	1.00 18.79	
	ATOM	477	CA		A 130	53.22		8.454	1.00 20.10	
25										
35	ATOM	478	СВ		A 130	52.63		7.183	1.00 19.92	
	MOTA	479	CG		A 130	51.35		6.708	1.00 27.85	
	ATOM	480	CD	GLU .	A 130	50.58	16.933	5.707	1.00 29.72	A
	MOTA	481	OE1	GLU .	A 130	51.21	.6 17.528	4.814	1.00 33.46	A
	ATOM	482	OE2	GLU .	A 130	49.33	9 16.996	5.807	1.00 30.74	A
40	ATOM	483	С		A 130	53.30	14.615	8.295	1.00 19.81	. А
	ATOM	484	0		A 130	52.55		8.935	1.00 18.37	
									1.00 20.41	_
	ATOM	485	N		A 131	54.21		7.447		
	ATOM	486	CA		A 131			7.202	1.00 22.45	
	ATOM	487	СВ	ARG .	A 131	55.44		6.098	1.00 25.16	a A
45	MOTA	488	CG	ARG .	A 131	55.74	2 11.043	5.840	1.00 28.75	A
	ATOM	489	CD	ARG .	A 131	56.73	6 10.837	4.708	1.00 33.75	A
	MOTA	490	NE	ARG	A 131			4.520	1.00 40.07	
	ATOM	491	CZ		A 131			3.532	1.00 43.07	
50	ATOM	492		ARG .				2.625	1.00 44.91	
50	MOTA	493		ARG .				3.449	1.00 44.45	
	MOTA	494	С	ARG .	A 131	54.82	11.982	8.466	1.00 23.24	A
	ATOM	495	0	ARG .	A 131	54.24	1 10.948	8.804	1.00 23.86	A
	ATOM	496	N		A 132	55.83		9.160	1.00 21.99	A
	ATOM	497	CA		A 132	56.31		10.370	1.00 22.04	
55		498			4 132 4 132					
55	ATOM		CB			57.57		10.888	1.00 23.72	
	ATOM	499	CG		A 132	58.75		9.932	1.00 27.77	
	MOTA	500		ASP .		58.68		8.989	1.00 27.34	
	MOTA	501	OD2	ASP .	A 132	59.75	3 13.163	10.128	1.00 28.70	A
	ATOM	502	С	ASP .	A 132	55.25	11.772	11.474	1.00 21.69	A

	ATOM	503	0	ASP	Α	132	55.077	10.723	12.092	1.00	22.75	A
	ATOM	504	N	VAL			54.551	12.868	11.725		19.54	A
		505		VAL			53.525	12.843	12.759		18.52	
	ATOM		CA									A
	MOTA	506	СВ	VAL			52.908	14.244	12.990		19.26	A
5	MOTA	507	CG1	VAL	Α	133	51.708	14.135	13.918	1.00	18.79	A
	ATOM	508	CG2	VAL	Α	133	53.953	15.180	13.604	1.00	18.80	A
	ATOM	509	С	VAL	Α	133	52.419	11.854	12.398	1.00	19.46	А
	ATOM	510	0	VAL			52.073	10.991	13.200		19.94	A
	ATOM	511		MET			51.878	11.957	11.187		19.15	A
10			N									
10	ATOM	512	CA	MET			50.807	11.052	10.792		21.25	A
	ATOM	513	СВ	MET			50.309	11.381	9.383		17.34	A
	MOTA	514	CG	MET	Α	134	49.615	12.730	9.302	1.00	20.00	A
	MOTA	515	SD	MET	Α	134	48.643	12.952	7.798	1.00	24.21	A
	ATOM	516	CE	MET	Α	134	47.033	12.434	8.400	1.00	23.20	А
15	ATOM	517	С	MET			51.203	9.582	10.881		22.43	А
13	ATOM	518	0	MET			50.384	8.741	11.249		23.82	A
	ATOM	519	N			135	52.454	9.273	10.556		23.09	A
	ATOM	520	CA			135	52.939	7.895	10.615		26.13	A
	ATOM	521	СВ	SER	Α	135	54.356	7.798	10.039	1.00	26.17	A
20	MOTA	522	OG	SER	Α	135	54.383	8.177	8.673	1.00	31.91	A
	ATOM	523	С	SER	Α	135	52.957	7.358	12.045	1.00	26.58	A
	ATOM	524	0	SER	Α	135	52.926	6.148	12.261	1.00	26.42	А
	ATOM	525	N	ARG			53.014	8.261	13.018		25.65	А
	ATOM	526	CA	ARG			53.056	7.870	14.425		27.47	A
25	ATOM	527	CB	ARG			53.823	8.914	15.238		27.97	A
23												
	ATOM	528	CG	ARG			55.283	9.082	14.857		32.00	A
	ATOM	529	CD	ARG			55.904	10.218	15.664		33.03	A
	MOTA	530	NE	ARG	Α	136	55.602	10.073	17.084	1.00	36.11	A
	ATOM	531	CZ	ARG	Α	136	55.867	10.990	18.007	1.00	39.74	A
30	ATOM	532	NH1	ARG	Α	136	56.449	12.132	17.661	1.00	40.55	A
	ATOM	533	NH2	ARG	Α	136	55.540	10.769	19.276	1.00	36.72	A
	ATOM	534	С	ARG	Ά	136	51.667	7.709	15.036	1.00	26.38	А
	ATOM	535	0	ARG			51.516	7.121	16.106		27.06	A
	ATOM	536	N	LEU			50.655	8.235	14.360		24.77	A
25												
35	ATOM	537	CA	LEU			49.294	8.162	14.870		24.70	A
	MOTA	538	СВ	LEU			48.483	9.363	14.371		24.52	A
	ATOM	539	CG	LEU	Α	137	49.050	10.760	14.662	1.00	26.67	A
	ATOM	540	CD1	LEU	Α	137	48.075	11.813	14.141	1.00	27.25	A
	MOTA	541	CD2	LEU	Α	137	49.279	10.945	16.155	1.00	27.09	A
40	ATOM	542	С	LEU	Α	137	48.592	6.868	14.473	1.00	25.20	А
	ATOM	543	0	LEU			48.619	6.469	13.309		25.99	А
	ATOM	544	N	ASP			47.971	6.218	15.451		21.89	A
	ATOM	545	CA	ASP			47.239	4.977	15.219		21.35	A
4.5	ATOM	546	CB	ASP			48.124	3.761	15.523		22.14	A
45	ATOM	547	CG	ASP			47.432	2.448	15.201		24.90	A
	ATOM	548		ASP			46.631	2.423	14.241	1.00	24.78	A
	MOTA	549	OD2	ASP	Α	138	47.691	1.443	15.897	1.00	25.39	A
	MOTA	550	С	ASP	Α	138	46.031	4.991	16.138	1.00	20.47	A
	ATOM	551	0	ASP	Α	138	45.967	4.248	17.118	1.00	19.06	A
50	ATOM	552	N	HIS			45.075	5.852	15.810		18.27	А
	ATOM	553	CA	HIS			43.869	6.016	16.606		18.21	A
	ATOM	554	CB	HIS			44.096	7.157	17.612		15.84	A
	MOTA	555	CG	HIS			42.985	7.332	18.600		15.24	A
	ATOM	556		HIS			42.884	6.964	19.900		13.97	A
55	ATOM	557		HIS			41.791	7.943	18.280		14.74	A
	MOTA	558	CE1	HIS	Α	139	41.002	7.944	19.341	1.00	14.19	A
	ATOM	559	NE2	HIS	Α	139	41.641	7.356	20.336	1.00	14.15	А
	ATOM	560	С	HIS			42.715	6.330	15.654		18.50	А
	ATOM	561	0	HIS			42.879	7.080	14.693		20.80	A
	111 011	O O T	~	1110	- 1		12.075	, . 000	11.000	1.00		

	ATOM	562	N	PRO .	A :	140	4	1.527	5.767	15.913	1.00	18.32	A
	ATOM	563	CD	PRO	ΖΔ .	140	4	1.143	4.984	17.100	1 00	16.71	А
	ATOM	564	CA	PRO .				0.367	6.001	15.048		17.43	A
	MOTA	565	CB	PRO .	Α.	140	3	9.273	5.157	15.704	1.00	16.64	A
5	ATOM	566	CG	PRO .	Α :	140	3	9.643	5.204	17.152	1.00	18.43	A
	ATOM	567	С	PRO				9.914	7.441	14.803		18.77	А
	ATOM	568	0	PRO				9.207	7.695	13.831		19.88	A
	MOTA	569	N	PHE	Α :	141	4	0.301	8.381	15.664		17.14	A
	ATOM	570	CA	PHE	Α :	141	3	9.874	9.767	15.477	1.00	16.42	A
10	ATOM	571	СВ	PHE	Δ.	141	3	9.568	10.422	16.836		14.60	А
10													
	MOTA	572	CG	PHE				8.386	9.817	17.556		15.26	A
	ATOM	573	CD1	PHE	Α.	141	3	7.335	9.234	16.842	1.00	14.78	A
	ATOM	574	CD2	PHE	Α :	141	3	8.297	9.880	18.942	1.00	13.70	A
	ATOM	575	CE1	PHE	Α.	141	3	6.215	8.727	17.502	1.00	16.94	А
15	ATOM	576		PHE				7.178	9.375	19.615		15.75	A
13													
	ATOM	577	CZ	PHE				6.135	8.799	18.893		16.89	А
	MOTA	578	С	PHE	Α :	141	4	0.857	10.641	14.694	1.00	16.15	A
	ATOM	579	0	PHE	Α :	141	4	0.799	11.871	14.761	1.00	17.35	A
	ATOM	580	N	PHE			4	1.748	10.011	13.941	1 00	15.88	А
20								2.727				17.89	
20	ATOM	581	CA	PHE					10.756	13.154			A
	ATOM	582	СВ	PHE			4	4.115	10.645	13.793		17.57	A
	ATOM	583	CG	PHE	A :	142	4	4.240	11.371	15.103	1.00	18.74	A
	ATOM	584	CD1	PHE	Α.	142	4	4.559	12.726	15.135	1.00	17.77	A
	ATOM	585		PHE				3.997	10.711	16.304		18.74	A
25													
25	ATOM	586		PHE				4.632	13.417	16.347		15.77	A
	MOTA	587	CE2	PHE	A :	142	4	4.065	11.393	17.522	1.00	17.56	A
	ATOM	588	CZ	PHE	Α :	142	4	4.383	12.747	17.542	1.00	17.14	A
	ATOM	589	С	PHE	Α.	142	4	2.793	10.231	11.729	1.00	19.12	А
	ATOM	590	0	PHE				2.659	9.030	11.504		20.01	A
30													
30	ATOM	591	N	VAL				2.978	11.135	10.769		18.72	A
	MOTA	592	$^{\rm CA}$	VAL .	A :	143	4	3.102	10.735	9.371	1.00	18.52	A
	ATOM	593	СВ	VAL	Α :	143	4	3.294	11.961	8.440	1.00	20.66	A
	ATOM	594	CG1	VAL .	Δ.	143	4	3.843	11.521	7.080	1.00	21.29	A
	ATOM	595		VAL				1.958	12.673	8.252		22.97	A
2.5													
35	MOTA	596	С	VAL				4.342	9.865	9.330		18.68	A
	MOTA	597	0	VAL .	A :	143	4	5.355	10.199	9.943	1.00	18.42	A
	ATOM	598	N	LYS	A :	144	4	4.259	8.745	8.623	1.00	18.30	A
	ATOM	599	CA	LYS	Α.	144	4	5.384	7.824	8.535	1.00	18.78	A
	ATOM	600	СВ	LYS				4.889	6.373	8.608		22.27	A
40													
40	MOTA	601	CG	LYS				6.017	5.340	8.557		29.72	A
	MOTA	602	CD	LYS .	A :	144	4	5.491	3.912	8.674	1.00	34.16	A
	ATOM	603	CE	LYS	A :	144	4	6.631	2.896	8.577	1.00	37.67	A
	ATOM	604	NZ	LYS	Α.	144	4	6.138	1.484	8.629	1.00	39.02	A
	ATOM	605	C	LYS				6.192	8.002	7.261		18.53	A
15													
45	ATOM	606	0	LYS				5.643	8.314	6.200		18.18	A
	MOTA	607	N	LEU .	Α :	145	4	7.502	7.816	7.385	1.00	16.79	A
	ATOM	608	CA	LEU	A :	145	4	8.411	7.900	6.251	1.00	17.45	A
	ATOM	609	СВ	LEU				9.686	8.653	6.641		18.82	A
50	ATOM	610	CG	LEU.				0.734	8.902	5.549		20.23	A
50	ATOM	611	CD1	LEU	Α.	145		1.836	9.799	6.093	1.00	18.83	A
	ATOM	612	CD2	LEU .	Α :	145	5	1.317	7.581	5.069	1.00	19.79	A
	ATOM	613	С	LEU	A :	145		8.739	6.450	5.907	1.00	19.19	А
	ATOM	614	0	LEU				9.451	5.772	6.659		17.36	A
	MOTA	615	N	TYR				8.215	5.972	4.782		17.28	A
55	ATOM	616	CA	TYR	Α :	146	4	8.444	4.593	4.358	1.00	17.57	A
	ATOM	617	СВ	TYR	Α :	146	4	7.288	4.098	3.486	1.00	17.74	А
	ATOM	618	CG	TYR				5.981	3.926	4.214		17.50	А
	ATOM	619		TYR				5.099	4.995	4.377		16.50	A
	ATOM	620	CEl	TYR	Α .	⊥46	4	3.881	4.827	5.039	1.00	17.10	A

	ATOM	621	CD2	TYR .	A 146	45.620	2.686	4.735	1.00 18.28	A
	ATOM	622	CE2	TYR .	A 146	44.411	2.506	5.399	1.00 19.84	A
	ATOM	623	CZ	TYR	A 146	43.547	3.576	5.544	1.00 17.53	A
	ATOM	624	OH		A 146		3.376	6.169	1.00 20.67	A
5		625	C					3.582	1.00 20.07	
3	ATOM				A 146		4.376			A
	ATOM	626	0		A 146		3.338	3.715	1.00 19.51	A
	ATOM	627	N	PHE .	A 147		5.350	2.765	1.00 18.09	A
	MOTA	628	CA	PHE .	A 147	51.307	5.203	1.952	1.00 17.20	A
	ATOM	629	СВ	PHE .	A 147	51.007	4.258	0.783	1.00 16.77	A
10	ATOM	630	CG	PHE .	A 147	49.835	4.699	-0.070	1.00 17.75	A
	ATOM	631	CD1	PHE .	A 147	49.967	5.752	-0.975	1.00 16.58	A
	ATOM	632		PHE .			4.075	0.053	1.00 18.07	А
	ATOM	633		PHE .			6.178	-1.742	1.00 19.62	A
	ATOM	634		PHE .			4.492	-0.710	1.00 18.56	A
1.5										
15	ATOM	635	CZ		A 147		5.546	-1.610	1.00 19.27	A
	ATOM	636	С		A 147		6.533	1.395	1.00 17.13	A
	MOTA	637	0	PHE .	A 147	51.045	7.528	1.452	1.00 14.43	A
	MOTA	638	N	THR .	A 148	52.981	6.534	0.854	1.00 17.12	A
	MOTA	639	CA	THR .	A 148	53.541	7.718	0.232	1.00 17.96	A
20	ATOM	640	СВ	THR .	A 148	54.449	8.531	1.197	1.00 21.51	A
	ATOM	641	OG1	THR .	A 148	55.605	7.760	1.537	1.00 18.83	A
	ATOM	642		THR .			8.897	2.472	1.00 19.60	A
	ATOM	643	C		A 148	54.386	7.262	-0.946	1.00 20.31	A
									1.00 20.31	
25	ATOM	644	0		A 148		6.124	-0.991		A
25	ATOM	645	N		A 149		8.149	-1.916	1.00 19.16	A
	ATOM	646	CA		A 149		7.877	-3.073	1.00 18.01	A
	MOTA	647	СВ	PHE .	A 149	54.748	6.801	-3.989	1.00 17.23	A
	ATOM	648	CG	PHE .	A 149	53.389	7.144	-4.544	1.00 16.88	A
	ATOM	649	CD1	PHE .	A 149	53.262	7.888	-5.712	1.00 18.58	A
30	ATOM	650	CD2	PHE .	A 149	52.235	6.668	-3.927	1.00 17.31	A
	ATOM	651		PHE .			8.149	-6.267	1.00 19.26	А
	ATOM	652		PHE .			6.923	-4.470	1.00 19.17	A
	ATOM	653	CZ		A 149		7.663	-5.642	1.00 19.17	A
2.5	ATOM	654	С		A 149		9.205	-3.774	1.00 20.85	A
35	ATOM	655	0		A 149		10.200	-3.376	1.00 19.76	A
	MOTA	656	N		A 150		9.241	-4.782	1.00 19.79	A
	ATOM	657	CA	GLN .	A 150	56.636	10.481	-5.497	1.00 24.03	A
	MOTA	658	СВ	GLN .	A 150	57.659	11.347	-4.739	1.00 24.45	A
	MOTA	659	CG	GLN .	A 150	58.986	10.645	-4.414	1.00 26.28	A
40	ATOM	660	CD	GLN .	A 150	59.988	11.558	-3.692	1.00 29.02	A
	ATOM	661	OE1	GLN .	A 150	60.693	12.353	-4.321	1.00 27.05	A
	ATOM	662		GLN .			11.449	-2.365	1.00 26.47	A
	ATOM	663	C		A 150		10.203	-6.885	1.00 23.88	A
	ATOM	664			A 150		9.118	-7.158	1.00 24.79	
15			0							A
45	ATOM	665	N	ASP.			11.171	-7.774	1.00 25.88	A
	ATOM	666	CA	ASP .			11.047	-9.117	1.00 26.49	A
	MOTA	667	СВ	ASP .	A 151	56.437	11.126	-10.199	1.00 24.54	A
	MOTA	668	CG	ASP .	A 151	55.544	12.336	-10.064	1.00 24.95	A
	ATOM	669	OD1	ASP .	A 151	56.005	13.379	-9.561	1.00 22.44	A
50	ATOM	670		ASP .				-10.490	1.00 25.72	А
	ATOM	671	С	ASP .			12.203	-9.220	1.00 28.63	A
	ATOM	672	0	ASP.			12.780	-8.194	1.00 27.83	A
				ASP .						
	ATOM	673	N					-10.426	1.00 29.21	A
	ATOM	674	CA	ASP.				-10.562	1.00 31.88	A
55	ATOM	675	СВ	ASP.				-12.026	1.00 33.94	A
	ATOM	676	CG	ASP .				-12.557	1.00 38.88	A
	ATOM	677		ASP .				-11.791	1.00 39.67	A
	MOTA	678	OD2	ASP .	A 152	60.817	12.211	-13.738	1.00 41.57	A
	ATOM	679	С	ASP .	A 152	59.487	14.994	-10.013	1.00 30.90	А

	ATOM	680	0	ASP	А	152	60.316	15.735	-9.482	1.00	31.69	А
	ATOM	681	N	GLU			58.207		-10.107		29.44	A
	ATOM	682	CA	GLU			57.767	16.632	-9.646		28.69	A
	ATOM	683	CB	GLU			56.984		-10.766		32.90	A
5	ATOM	684	CG	GLU			57.451		-12.183		40.57	A
J	ATOM	685	CD	GLU			56.920		-12.103		45.78	A
		686							-12.873 -12.760		48.91	
	ATOM			GLU			55.682					A
	ATOM	687		GLU			57.736		-12.979		48.95	A
1.0	ATOM	688	С	GLU			56.929	16.683	-8.372		26.43	A
10	ATOM	689	0	GLU			56.947	17.688	-7.660		25.08	A
	ATOM	690	N	LYS			56.205	15.610	-8.069		22.39	A
	ATOM	691	CA	LYS			55.318	15.631	-6.912		21.43	А
	ATOM	692	СВ	LYS			53.861	15.628	-7.398		20.33	A
	ATOM	693	CG	LYS			53.505	16.716	-8.403		21.92	A
15	ATOM	694	CD	LYS			52.211	16.375	-9.146		19.70	A
	MOTA	695	CE	LYS	А	154	51.775	17.503	-10.077	1.00	20.04	A
	ATOM	696	NZ	LYS	Α	154	50.631	17.094	-10.951	1.00	19.97	A
	ATOM	697	С	LYS	Α	154	55.458	14.522	-5.881	1.00	20.43	A
	ATOM	698	0	LYS	Α	154	55.949	13.426	-6.173	1.00	21.13	A
20	ATOM	699	N	LEU	Α	155	54.985	14.832	-4.676	1.00	19.69	A
	ATOM	700	CA	LEU	Α	155	54.950	13.900	-3.553	1.00	19.10	А
	ATOM	701	СВ	LEU	Α	155	55.362	14.588	-2.252		19.65	А
	ATOM	702	CG	LEU			56.740	15.234	-2.129		21.20	А
	ATOM	703		LEU			56.848	15.918	-0.770		23.42	A
25	ATOM	704		LEU			57.816	14.174	-2.277		23.08	A
23	ATOM	705	C	LEU			53.478	13.507	-3.427		18.87	A
	ATOM	706	0	LEU			52.600	14.348	-3.620		18.61	A
	ATOM	707	N			156	53.209	12.249	-3.091		15.02	A
		708		TYR			51.834	11.783	-2.934		16.29	A
30	ATOM	708	CA	TYR				10.769	-2.934 -4.029		14.20	A
30	ATOM		CB				51.470					
	ATOM	710	CG	TYR			51.603	11.273	-5.449		17.29	A
	ATOM	711		TYR			52.857	11.429	-6.045		16.46	A
	ATOM	712		TYR			52.978	11.884	-7.360		18.68	A
	ATOM	713	CD2				50.474	11.588	-6.202		16.43	A
35	ATOM	714	CE2	TYR			50.583	12.048	-7.512		16.31	A
	ATOM	715	CZ	TYR			51.835	12.192	-8.083		18.17	A
	ATOM	716	OH	TYR			51.941	12.651	-9.371		17.47	A
	ATOM	717	С	TYR			51.657	11.108	-1.572		16.32	A
	ATOM	718	0	TYR			52.412	10.197	-1.235		16.27	A
40	ATOM	719	N	PHE	Α	157	50.678	11.568	-0.792	1.00	15.47	A
	MOTA	720	CA	PHE	Α	157	50.385	10.966	0.508	1.00	16.66	A
	ATOM	721	СВ	PHE	Α	157	50.324	12.014	1.629	1.00	16.91	A
	MOTA	722	CG	PHE	Α	157	51.631	12.708	1.907	1.00	18.96	A
	ATOM	723	CD1	PHE	Α	157	52.821	12.261	1.340	1.00	20.31	A
45	ATOM	724	CD2	PHE	Α	157	51.664	13.829	2.732	1.00	21.12	A
	ATOM	725		PHE			54.025	12.926	1.585		22.08	А
	ATOM	726		PHE			52.865	14.500	2.982		22.18	A
	ATOM	727	CZ	PHE			54.045	14.045	2.405		21.27	А
	ATOM	728	С	PHE			49.016	10.308	0.404		16.52	А
50	ATOM	729	0	PHE			48.029	10.979	0.110		17.32	A
20	ATOM	730	N	GLY			48.953	9.002	0.644		15.97	A
	ATOM	731	CA	GLY			47.684	8.299	0.572		16.13	A
	ATOM	732	C	GLY			47.004	8.383	1.920		14.94	A
	ATOM	733	0	GLY			47.445	7.756	2.879		16.28	A
55												
ככ	ATOM	734	N	LEU			45.915	9.145	1.989		13.50	A
	ATOM	735	CA	LEU			45.191	9.340	3.241		15.20	A
	ATOM	736	CB	LEU			45.031	10.835	3.517		14.20	A
	ATOM	737	CG	LEU			46.270	11.726	3.385		19.00	A
	ATOM	738	CDI	LEU	А	159	45.847	13.188	3.477	T.00	17.12	А

	ATOM	739	CD2	LEU 2	159	47.275	11.390	4.471	1.00 14.71	A
	ATOM	740	С	LEU :	A 159	43.809	8.716	3.232	1.00 15.53	А
	ATOM	741	0		159	43.232	8.472	2.177	1.00 16.05	A
	ATOM	742	N		160	43.268	8.469	4.418	1.00 15.86	A
5	MOTA	743	CA		160	41.932	7.917	4.498	1.00 19.01	A
	MOTA	744	СВ	SER 2	160	41.566	7.582	5.949	1.00 22.90	A
	ATOM	745	OG	SER I	160	41.901	8.629	6.833	1.00 24.18	A
	ATOM	746	С		160	40.987	8.968	3.924	1.00 20.43	A
	ATOM	747	0		1 160	41.213	10.173	4.062	1.00 19.96	A
10										
10	ATOM	748	N		A 161	39.945	8.508	3.250	1.00 19.20	A
	ATOM	749	CA		161	38.975	9.406	2.644	1.00 20.37	A
	MOTA	750	СВ	TYR 2	161	38.471	8.785	1.332	1.00 20.00	A
	ATOM	751	CG	TYR I	161	37.314	9.502	0.666	1.00 20.72	A
	ATOM	752	CD1	TYR 2	161	37.222	10.895	0.682	1.00 18.22	А
15	ATOM	753		TYR		36.180	11.557	0.029	1.00 22.24	A
13										
	ATOM	754		TYR Z		36.333	8.784	-0.020	1.00 20.53	A
	MOTA	755		TYR 2		35.287	9.436	-0.678	1.00 24.24	A
	MOTA	756	CZ	TYR .	161	35.218	10.822	-0.648	1.00 22.32	A
	MOTA	757	OH	TYR 2	161	34.194	11.471	-1.298	1.00 23.03	A
20	ATOM	758	С	TYR Z	161	37.812	9.681	3.598	1.00 20.14	A
	ATOM	759	0		A 161	36.959	8.819	3.810	1.00 19.53	А
	ATOM	760	N		162	37.791	10.880	4.178	1.00 19.92	A
	MOTA	761	CA		162	36.721	11.271	5.099	1.00 21.07	A
	ATOM	762	СВ		162	37.187	12.419	6.002	1.00 19.60	A
25	ATOM	763	С	ALA 2	162	35.542	11.712	4.238	1.00 22.07	A
	MOTA	764	0	ALA 2	162	35.436	12.875	3.860	1.00 20.66	A
	ATOM	765	N	LYS 2	163	34.653	10.769	3.945	1.00 23.27	A
	ATOM	766	CA	LYS 2	A 163	33.503	11.017	3.080	1.00 27.12	A
	ATOM	767	СВ		163	32.663	9.741	2.963	1.00 29.68	А
30	ATOM	768	CG		163	33.455	8.524	2.515	1.00 37.67	A
30		769			1 163				1.00 42.24	
	ATOM		CD			32.556	7.310	2.321		A
	ATOM	770	CE		163	33.373	6.034	2.185	1.00 44.48	A
	MOTA	771	NZ		163	34.143	5.735	3.430	1.00 44.88	A
	MOTA	772	С	LYS 2	163	32.581	12.186	3.411	1.00 25.78	A
35	MOTA	773	0	LYS 2	163	32.103	12.863	2.506	1.00 26.53	A
	ATOM	774	N	ASN I	164	32.327	12.441	4.689	1.00 24.57	A
	ATOM	775	CA	ASN	164	31.420	13.522	5.033	1.00 23.77	А
	ATOM	776	СВ		164	30.610	13.129	6.265	1.00 25.02	A
	ATOM	777	CG		1 164	29.537	12.101	5.932	1.00 23.02	A
40										
40	MOTA	778		ASN Z		28.772	12.281	4.983	1.00 28.79	A
	MOTA	779		ASN 2		29.475	11.024	6.704	1.00 27.13	A
	MOTA	780	С	ASN 2	164	31.999	14.931	5.169	1.00 24.43	A
	MOTA	781	0	ASN 2	164	31.306	15.856	5.589	1.00 23.98	A
	ATOM	782	N	GLY I	165	33.262	15.097	4.795	1.00 21.56	A
45	ATOM	783	CA	GLY I	165	33.873	16.414	4.836	1.00 24.39	A
	ATOM	784	С		A 165	34.191	17.043	6.181	1.00 23.62	А
	ATOM	785	0		1 165	34.380	16.352	7.177	1.00 23.26	
										A
	ATOM	786	N		166	34.234	18.373	6.186	1.00 23.22	A
	MOTA	787	CA		166	34.563	19.176	7.362	1.00 24.54	A
50	ATOM	788	СВ	GLU 1	166	35.055	20.558	6.913	1.00 25.04	A
	MOTA	789	CG	GLU Z	166	36.419	20.569	6.229	1.00 26.48	A
	ATOM	790	CD	GLU I	166	36.699	21.889	5.517	1.00 30.02	А
	ATOM	791		GLU Z		36.081	22.906	5.889	1.00 29.33	А
	ATOM	792		GLU I		37.544	21.916	4.596	1.00 20.33	A
55										
55	ATOM	793	C		166	33.436	19.372	8.369	1.00 24.44	A
	MOTA	794	0		166	32.279	19.541	8.001	1.00 22.76	A
	MOTA	795	N		167	33.791	19.370	9.649	1.00 22.95	A
	ATOM	796	CA	LEU Z	167	32.813	19.581	10.707	1.00 22.26	A
	ATOM	797	СВ	LEU 2	167	33.497	19.481	12.073	1.00 22.32	A

	ATOM	798	CG	LEU A			32.706	19.923	13.306		22.04	А
	MOTA	799		LEU A			31.454	19.074	13.463		19.66	A
	MOTA	800		LEU A			33.597	19.805	14.537		21.17	A
	MOTA	801	С	LEU A			32.193	20.971	10.529		23.49	A
5	MOTA	802	0	LEU A			31.047	21.209	10.907		23.56	A
	MOTA	803	N	LEU A	168		32.960	21.887	9.948		24.25	A
	ATOM	804	CA	LEU A	168		32.473	23.245	9.722	1.00	26.64	A
	ATOM	805	СВ	LEU A	168		33.560	24.099	9.066	1.00	25.62	A
	ATOM	806	CG	LEU A	168	:	33.198	25.546	8.707	1.00	27.34	A
10	ATOM	807	CD1	LEU A	168		32.718	26.296	9.946	1.00	26.42	A
	ATOM	808	CD2	LEU A	168	;	34.418	26.238	8.119	1.00	26.74	A
	ATOM	809	С	LEU A	168		31.234	23.218	8.829	1.00	27.13	A
	ATOM	810	0	LEU A	168		30.297	23.989	9.030	1.00	26.01	A
	ATOM	811	N	LYS A			31.233	22.320	7.848		26.41	A
15	ATOM	812	CA	LYS A			30.106	22.210	6.934		27.70	А
	ATOM	813	СВ	LYS A			30.324	21.064	5.945		30.49	А
	ATOM	814	CG	LYS A			29.151	20.854	4.993		32.47	A
	ATOM	815	CD	LYS A			29.407	19.728	3.998		35.98	A
	ATOM	816	CE	LYS A			29.462	18.372	4.683		38.53	A
20	ATOM	817	ΝZ	LYS A			29.622	17.263	3.702		41.00	A
20	ATOM	818	C	LYS A			28.801	21.985	7.682		28.12	A
	ATOM	819	0	LYS A			27.785	22.608	7.371		28.08	A
	ATOM	820	N	TYR A			28.826	21.094	8.668		26.53	A
	ATOM	821	CA	TYR A			27.624	20.791	9.434		26.95	A
25	ATOM	822	CB	TYR A			27.810	19.476	10.193		25.03	A
23	ATOM	823	CG	TYR A			27.818	18.300	9.251		26.65	A
	ATOM	824	CD1				26.745	17.661	8.790		28.27	
			CE1					16.642	7.839			A
	ATOM	825					26.814				26.85	A
30	ATOM	826	CD2				29.127	17.884	8.742		27.83	A
30	ATOM	827	CE2	TYR A			29.209	16.869	7.792		27.19	A
	ATOM	828	CZ	TYR A			28.049	16.254	7.343		30.02	A
	ATOM	829	OH	TYR A			28.130	15.268	6.382		29.23	A
	ATOM	830	С	TYR A			27.229	21.918	10.376		27.59	A
2.5	ATOM	831	0	TYR A			26.045	22.122	10.642		29.25	A
35	ATOM	832	N	ILE A			28.208	22.660	10.882		28.16	A
	MOTA	833	CA	ILE A			27.883	23.770	11.763		29.03	A
	ATOM	834	СВ	ILE A			29.151	24.435	12.337		27.51	A
	ATOM	835	CG2	ILE A			28.773	25.705	13.084		27.97	A
	MOTA	836	CG1	ILE A			29.872	23.458	13.272		26.70	A
40	MOTA	837	CD1				31.163	23.996	13.856		24.07	A
	MOTA	838	С	ILE A			27.094	24.796	10.944		31.41	A
	MOTA	839	0	ILE A			26.088	25.335	11.407		31.69	A
	MOTA	840	N	ARG A			27.546	25.047	9.719		33.21	A
	MOTA	841	CA	ARG A			26.874	26.000	8.844		36.54	A
45	ATOM	842	СВ	ARG A			27.734	26.314	7.616		37.73	A
	ATOM	843	CG	ARG A			29.057	27.011	7.912		41.65	A
	MOTA	844	CD	ARG A			29.708	27.492	6.616		45.29	A
	MOTA	845	NE	ARG A			31.037	28.070	6.812		48.51	A
	ATOM	846	CZ	ARG A			31.314	29.059	7.658	1.00	51.53	A
50	ATOM	847		ARG A			30.355	29.593	8.406	1.00	53.75	A
	ATOM	848	NH2	ARG A			32.553	29.526	7.748		51.21	A
	ATOM	849	С	ARG A		:	25.528	25.459	8.378	1.00	37.67	A
	MOTA	850	0	ARG A		:	24.550	26.200	8.288	1.00	39.09	A
	ATOM	851	N	LYS A	173	:	25.481	24.163	8.092	1.00	38.44	A
55	ATOM	852	CA	LYS A	173	:	24.259	23.528	7.619	1.00	39.25	А
	ATOM	853	СВ	LYS A	173	:	24.523	22.061	7.272		41.89	A
	ATOM	854	CG	LYS A	173	:	23.279	21.298	6.830	1.00	45.52	A
	ATOM	855	CD	LYS A	173	:	23.557	19.808	6.653	1.00	49.60	A
	MOTA	856	CE	LYS A	173	:	24.477	19.530	5.469	1.00	52.63	A

	ATOM	857	NZ	LYS	Α	173	23.855	19.894	4.160	1.00	54.61	Α
	ATOM	858	С	LYS	Α	173	23.089	23.608	8.595	1.00	39.30	A
	MOTA	859	0	LYS	A	173	21.981	23.960	8.201	1.00	39.62	A
	MOTA	860	N	ILE	Α	174	23.320	23.282	9.863	1.00	37.96	Α
5	MOTA	861	CA	ILE	Α	174	22.229	23.314	10.833		37.36	A
	MOTA	862	СВ	ILE	Α	174	22.159	21.998	11.652		37.44	А
	MOTA	863	CG2	ILE	Α	174	22.058	20.802	10.709	1.00	38.37	А
	MOTA	864	CG1	ILE	Α	174	23.397	21.850	12.532	1.00	37.25	А
	MOTA	865	CD1	ILE	Α	174	23.355	20.620	13.418	1.00	36.85	А
10	ATOM	866	С	ILE	Α	174	22.259	24.492	11.801		36.71	А
	MOTA	867	0	ILE			21.448	24.556	12.724		38.05	Α
	MOTA	868	N	GLY			23.185	25.423	11.592		35.48	А
	MOTA	869	CA	GLY			23.265	26.585	12.462		35.29	Α
	ATOM	870	С	GLY			24.053	26.360	13.737		35.06	А
15	ATOM	871	0	GLY			25.066	27.019	13.970		37.46	А
	ATOM	872	N	SER			23.581	25.441	14.571		33.94	А
	ATOM	873	CA	SER			24.253	25.113	15.822		32.84	А
	ATOM	874	СВ	SER			23.938	26.155	16.901		33.54	А
	ATOM	875	OG	SER			22.599	26.056	17.347		34.86	А
20	ATOM	876	С	SER			23.796	23.731	16.276		32.34	A
	ATOM	877	0	SER			22.726	23.263	15.884		32.82	A
	ATOM	878	N	PHE			24.609	23.085	17.103		29.39	Α
	ATOM	879	CA	PHE			24.313	21.743	17.597		27.20	A
2.5	ATOM	880	СВ	PHE			25.621	20.989	17.865		26.39	A
25	ATOM	881	CG	PHE			26.372	20.585	16.622		26.18	A
	ATOM	882		PHE			26.210	21.277	15.426		25.30	A
	ATOM	883		PHE			27.266	19.516	16.662		26.05	A
	ATOM	884		PHE			26.923	20.912	14.290		26.59	A
20	ATOM	885		PHE			27.986	19.143	15.532		26.06	A
30	ATOM	886	CZ	PHE			27.815	19.841	14.343		25.42	A
	ATOM	887	C	PHE			23.500	21.752	18.884		27.00	A
	ATOM	888	O NT	PHE			23.704	22.610	19.747		26.48	A
	MOTA	889	N	ASP ASP			22.578	20.802	19.022		26.70 26.35	A
35	ATOM	890 891	CA CB	ASP			21.816 20.621	19.773	20.260		29.90	A
33	ATOM ATOM	892	СБ	ASP			21.020	18.372	20.142		32.28	A A
	ATOM	893		ASP			22.157	17.949	20.014		35.21	A
	ATOM	894		ASP			20.179	17.683	19.105		34.79	A
	ATOM	895	C	ASP			22.810	20.228	21.311		25.03	A
40	ATOM	896	0	ASP			23.974	19.968	20.992		21.24	A
40	ATOM	897	N	GLU			22.361	20.083	22.552		23.60	A
	ATOM	898	CA	GLU			23.247	19.644	23.619		25.18	A
	ATOM	899	CB	GLU			22.542	19.770	24.971		27.60	A
	ATOM	900	CG	GLU			23.324	19.176	26.130		32.58	A
45	ATOM	901	CD	GLU			22.997	19.845	27.449		35.82	A
15	ATOM	902		GLU			21.825	20.224	27.645		35.95	A
	ATOM	903		GLU			23.912	19.984	28.291		38.19	A
	ATOM	904	C	GLU			23.808	18.235	23.450		24.08	A
	ATOM	905	0	GLU			24.977	17.989	23.756		22.79	A
50	ATOM	906	N	THR			22.983	17.316	22.961		23.36	A
	ATOM	907	CA	THR			23.412	15.935	22.761		22.15	Α
	ATOM	908	СВ	THR			22.224	15.054	22.320		23.77	А
	ATOM	909		THR			21.222	15.075	23.341		26.37	A
	ATOM	910		THR			22.670	13.616	22.088		22.66	A
55	ATOM	911	С	THR			24.533	15.830	21.724		22.01	A
	ATOM	912	0	THR			25.533	15.141	21.944		19.87	А
	MOTA	913	N	CYS			24.365	16.511	20.596		21.21	Α
	ATOM	914	CA	CYS			25.372	16.480	19.541		22.22	Α
	ATOM	915	СВ	CYS	Α	181	24.800	17.065	18.250		24.62	Α

	ATOM	916	SG	CYS	Α	181	23.435	16.080	17.560	1.00	29.50	A
	ATOM	917	С	CVS	Ζ	181	26.633	17.232	19.954	1.00	23 07	Α
	ATOM	918	0	CYS			27.746	16.827	19.608	1.00		A
	ATOM	919	N	THR	Α	182	26.463	18.325	20.695	1.00	22.76	Α
5	ATOM	920	CA	THR	Δ	182	27.606	19.103	21.161	1.00	21 49	Α
9												
	ATOM	921	СВ	THR			27.167	20.346	21.978	1.00		А
	ATOM	922	og1	THR	Α	182	26.459	21.262	21.134	1.00	22.50	Α
	ATOM	923	CG2	THR	Α	182	28.379	21.046	22.565	1.00	18.36	A
	ATOM	924	С	THR			28.454	18.215	22.071	1.00		A
10												
10	ATOM	925	0	THR	А	182	29.669	18.090	21.894	1.00	19.95	A
	ATOM	926	N	ARG	Α	183	27.798	17.602	23.050	1.00	18.97	A
	ATOM	927	CA	ARG	Δ	183	28.468	16.723	23.996	1.00	19 39	Α
				ARG								
	ATOM	928	СВ				27.455	16.140	24.984	1.00		А
	ATOM	929	CG	ARG	Α	183	28.030	15.062	25.887	1.00	18.77	Α
15	ATOM	930	CD	ARG	Α	183	27.021	14.571	26.925	1.00	21.19	Α
	ATOM	931	NE	ARG			26.605	15.642	27.824	1.00		Α
	ATOM	932	CZ	ARG	А	T83	25.496	16.362	27.679	1.00		Α
	ATOM	933	NH1	ARG	Α	183	24.672	16.123	26.666	1.00	19.81	Α
	ATOM	934	NH2	ARG	Α	183	25.224	17.338	28.539	1.00	17.11	Α
20				ARG				15.577				
20	ATOM	935	С				29.206		23.302	1.00		A
	ATOM	936	0	ARG	Α	183	30.383	15.333	23.573	1.00	19.97	Α
	ATOM	937	N	PHE	Α	184	28.520	14.871	22.409	1.00	19.24	А
	ATOM	938	CA	PHE			29.144	13.746	21.722	1.00		Α
	ATOM	939	СВ	PHE			28.158	13.078	20.764	1.00		Α
25	ATOM	940	CG	PHE	Α	184	28.719	11.857	20.098	1.00	22.67	Α
	ATOM	941	CD1	PHE	Α	184	28.717	10.630	20.754	1.00	22.97	A
		942		PHE			29.317	11.949	18.850	1.00		
	ATOM											A
	ATOM	943	CE1	PHE	Α	184	29.308	9.510	20.176	1.00	23.53	Α
	ATOM	944	CE2	PHE	Α	184	29.915	10.833	18.263	1.00	24.11	Α
30	ATOM	945	CZ	PHE			29.910	9.613	18.928	1.00	22 97	Α
50												
	ATOM	946	С	PHE			30.403	14.127	20.941	1.00		Α
	ATOM	947	0	PHE	Α	184	31.461	13.531	21.130	1.00	18.89	Α
	ATOM	948	N	TYR	Α	185	30.292	15.110	20.056	1.00	15.73	A
	ATOM	949	CA			185	31.443	15.519	19.265	1.00		A
2.5												
35	ATOM	950	СВ	TYR	А	182	30.992	16.413	18.111	1.00		Α
	MOTA	951	CG	TYR	Α	185	30.364	15.584	17.015	1.00	19.37	A
	ATOM	952	CD1	TYR	Д	185	31.159	14.809	16.168	1.00	16.53	Α
		953		TYR			30.590	13.952	15.232	1.00		A
	ATOM											
	ATOM	954	CD2	TYR	Α	185	28.976	15.484	16.892	1.00	18.18	Α
40	ATOM	955	CE2	TYR	Α	185	28.398	14.623	15.956	1.00	18.90	A
	ATOM	956	CZ	TYR	Δ	185	29.211	13.861	15.133	1.00	18 41	Α
	ATOM	957	OH	TYR			28.650	12.995	14.218	1.00		Α
	MOTA	958	С	TYR	Α	185	32.544	16.172	20.083	1.00	15.79	Α
	ATOM	959	0	TYR	Α	185	33.720	16.015	19.766	1.00	17.69	A
45	ATOM	960	N	THR			32.176	16.887	21.142	1.00		Α
73												
	ATOM	961	CA	THR	А	T80	33.184	17.504	21.997	1.00		Α
	ATOM	962	СВ	THR	Α	186	32.559	18.403	23.094	1.00	16.62	A
	ATOM	963	OG1	THR	Α	186	31.866	19.503	22.481	1.00	14.79	A
		964		THR								
50	ATOM						33.656	18.953	24.019	1.00		A
50	ATOM	965	С	THR	А	186	33.954	16.375	22.680	1.00	15.59	Α
	ATOM	966	0	THR	Α	186	35.176	16.443	22.823	1.00	13.77	A
	ATOM	967	N	ALA			33.234	15.333	23.097	1.00	14.06	Α
	ATOM	968	CA	ALA			33.869	14.196	23.757	1.00		A
	MOTA	969	СВ	ALA	Α	187	32.810	13.195	24.224	1.00	14.32	Α
55	ATOM	970	С	ALA	Α	187	34.875	13.509	22.821	1.00	14.41	Α
	ATOM	971	0	ALA			35.972	13.136	23.247	1.00		A
	ATOM	972	N	GLU			34.516	13.340	21.549	1.00		А
	ATOM	973	CA	GLU	Α	188	35.443	12.704	20.615	1.00	13.50	Α
	ATOM	974	СВ	GLU	Α	188	34.782	12.449	19.251	1.00		А
		-	_		_						-	

	ATOM	975	CG	CTII	7\	188	33.622	11.454	19.282	1.00 1	2 71	А
	ATOM	976	CD	GLU			33.464	10.685	17.979	1.00 1		A
	ATOM	977		GLU			33.687	11.275	16.899	1.00 1		A
_	ATOM	978		GLU			33.110	9.484	18.031	1.00 1		A
5	MOTA	979	С	GLU			36.682	13.582	20.436	1.00 1		A
	MOTA	980	0	GLU	Α	188	37.803	13.085	20.408	1.00 1		A
	MOTA	981	N	ILE	Α	189	36.486	14.893	20.326	1.00 1	3.52	A
	ATOM	982	CA	ILE	Α	189	37.627	15.787	20.159	1.00 1	3.35	A
	ATOM	983	СВ	ILE	Α	189	37.169	17.247	19.939	1.00 1	3.95	A
10	ATOM	984	CG2	ILE	Α	189	38.381	18.165	19.822	1.00 1	2.47	A
	ATOM	985		ILE			36.302	17.332	18.671	1.00 1		A
	ATOM	986		ILE			35.588	18.664	18.491	1.00 1		A
	ATOM	987	C			189	38.530	15.702	21.394	1.00 1		A
	ATOM	988	0			189	39.753	15.595	21.271	1.00 1		A
1.5												
15	ATOM	989	N			190	37.927	15.751	22.582	1.00 1		A
	ATOM	990	CA	VAL			38.684	15.655	23.832	1.00 1		A
	ATOM	991	СВ	VAL			37.743	15.690	25.061	1.00 1		A
	MOTA	992		VAL			38.509	15.267	26.326	1.00 1		A
	ATOM	993		VAL			37.160	17.082	25.233	1.00 1		А
20	MOTA	994	С			190	39.468	14.338	23.859	1.00 1		А
	MOTA	995	0	VAL	Α	190	40.634	14.304	24.250	1.00 1	3.72	A
	MOTA	996	N	SER	Α	191	38.825	13.254	23.432	1.00 1	5.26	A
	ATOM	997	CA	SER	Α	191	39.478	11.943	23.421	1.00 1	6.81	A
	ATOM	998	СВ	SER	Α	191	38.470	10.857	23.041	1.00 1	6.14	А
25	ATOM	999	OG	SER	Α	191	39.018	9.569	23.238	1.00 1	6.94	A
	ATOM	1000	С			191	40.649	11.928	22.441	1.00 1		A
	ATOM	1001	0			191	41.697	11.335	22.713	1.00 1		A
	ATOM	1002	N			192	40.468	12.586	21.300	1.00 1		A
	ATOM	1002	CA	ALA			41.518	12.645	20.292	1.00 1		A
30		1003	CB	ALA			40.989	13.296	19.016	1.00 1		A
30	ATOM											
	ATOM	1005	С	ALA			42.695	13.440	20.845	1.00 1		A
	ATOM	1006	0	ALA			43.851	13.038	20.697	1.00 1		A
	ATOM	1007	N			193	42.401	14.563	21.496	1.00 1		A
	ATOM	1008	CA	LEU			43.459	15.392	22.067	1.00 1		A
35	ATOM	1009	СВ	LEU	Α	193	42.884	16.712	22.600	1.00 1		A
	MOTA	1010	CG	LEU	Α	193	42.445	17.721	21.525	1.00 1	5.97	A
	ATOM	1011	CD1	LEU	Α	193	41.869	18.979	22.190	1.00 1	3.97	A
	MOTA	1012	CD2	LEU	Α	193	43.642	18.088	20.655	1.00 1	4.58	A
	MOTA	1013	С	LEU	Α	193	44.211	14.659	23.174	1.00 1	4.49	A
40	MOTA	1014	0	LEU	Α	193	45.427	14.813	23.310	1.00 1	6.56	A
	ATOM	1015	N	GLU	Α	194	43.500	13.870	23.975	1.00 1	3.96	A
	ATOM	1016	CA	GLU	Α	194	44.179	13.123	25.032	1.00 1	4.08	A
	ATOM	1017	СВ	GLU	Α	194	43.190	12.295	25.857	1.00 1	4.65	А
	ATOM	1018	CG	GLU			43.882	11.301	26.789	1.00 1		A
45	ATOM	1019	CD	GLU			42.924	10.592	27.730	1.00 1		A
7.5	ATOM	1020		GLU			41.809	10.237	27.735	1.00 1		A
				GLU			43.302					
	ATOM	1021						10.380	28.906	1.00 2		A
	ATOM	1022	С	GLU			45.208	12.199	24.386	1.00 1		A
50	ATOM	1023	0	GLU			46.337	12.093	24.847	1.00 1		A
50	ATOM	1024	N			195	44.822	11.544	23.301	1.00 1		A
	ATOM	1025	CA			195	45.743	10.642	22.618	1.00 1		A
	MOTA	1026	СВ	TYR	Α	195	45.030	9.910	21.488	1.00 1	7.29	А
	MOTA	1027	CG	TYR	А	195	45.956	9.058	20.649	1.00 1	7.92	A
	MOTA	1028	CD1	TYR	А	195	46.347	7.788	21.077	1.00 1	7.96	A
55	ATOM	1029	CE1	TYR	Α	195	47.203	6.996	20.304	1.00 1	9.77	A
	ATOM	1030	CD2	TYR	Α	195	46.445	9.524	19.428	1.00 1	6.67	A
	ATOM	1031		TYR			47.299	8.744	18.650	1.00 1		A
	ATOM	1032	CZ			195	47.671	7.481	19.094	1.00 2		A
	ATOM	1033	OH			195	48.506	6.705	18.325	1.00 2		A
					-	_					-	

	ATOM	1034	С	TYR	Α	195	46.917	11.419	22.035	1.00	16.98	А
	ATOM	1035	0	TYR	Α	195	48.081	11.047	22.203	1.00	14.61	А
	MOTA	1036	N	LEU	Α	196	46.599	12.507	21.347	1.00	16.30	A
	ATOM	1037	CA	LEU	Α	196	47.619	13.328	20.720	1.00	18.15	A
5	ATOM	1038	СВ	LEU	Α	196	46.969	14.502	19.982	1.00	18.59	A
	ATOM	1039	CG	LEU	Α	196	47.834	15.203	18.935	1.00	22.51	A
	ATOM	1040	CD1	LEU	Α	196	48.222	14.206	17.841	1.00	20.94	A
	ATOM	1041	CD2	LEU	Α	196	47.060	16.375	18.338	1.00	22.98	A
	MOTA	1042	С	LEU	Α	196	48.592	13.844	21.763	1.00	17.75	A
10	MOTA	1043	0	LEU	Α	196	49.801	13.644	21.649	1.00	18.33	A
	ATOM	1044	N	HIS			48.064	14.495	22.792		17.12	A
	ATOM	1045	CA	HIS			48.913	15.042	23.842		18.47	A
	ATOM	1046	СВ	HIS			48.069	15.866	24.817		15.90	A
	ATOM	1047	CG	HIS			47.571	17.152	24.231		19.15	A
15	MOTA	1048		HIS			47.830	17.745	23.038		18.22	A
	MOTA	1049		HIS			46.704	17.992	24.897		17.47	A
	MOTA	1050		HIS			46.450	19.047	24.139		19.74	A
	ATOM	1051		HIS			47.119	18.921	23.007		15.69	A
20	ATOM	1052	С	HIS			49.696	13.958	24.572		19.40	A
20	ATOM	1053	0	HIS			50.823	14.192	25.021		19.42	A
	ATOM	1054	N	GLY			49.106	12.770	24.679		18.59	A
	ATOM	1055	CA	GLY			49.793	11.675	25.339		19.60	A
	ATOM	1056	C	GLY			51.075	11.307	24.612		21.86	A
25	ATOM	1057	0	GLY			51.963	10.682	25.186		23.09	A
25	ATOM	1058	N	LYS			51.174 52.368	11.687	23.341		22.81	A
	ATOM	1059	CA			199		11.401	22.549		24.43	A
	MOTA	1060	CB	LYS			51.990 51.378	10.905 9.520	21.154		26.00	A
	ATOM	1061 1062	CG CD			199 199	51.291	9.002	21.133 19.708		36.85	A
30	ATOM ATOM	1062	CE	LYS			50.832	7.559	19.700		40.37	A A
30	ATOM	1063	NZ	LYS			51.646	6.691	20.581		43.48	A
	ATOM	1065	C	LYS			53.253	12.631	22.414		23.88	A
	ATOM	1066	0			199	54.144	12.669	21.568		24.97	A
	ATOM	1067	N			200	52.997	13.638	23.243		24.00	A
35	ATOM	1068	CA	GLY			53.790	14.853	23.203		22.12	A
	ATOM	1069	C			200	53.665	15.632	21.907		22.14	A
	ATOM	1070	0			200	54.632	16.231	21.439		22.41	A
	ATOM	1071	N			201	52.475	15.630	21.320		20.00	A
	ATOM	1072	CA			201	52.252	16.355	20.080		18.93	A
40	ATOM	1073	СВ			201	51.784	15.414	18.955		19.70	А
	ATOM	1074	CG2	ILE	Α	201	51.414	16.226	17.716	1.00	20.12	A
	ATOM	1075	CG1	ILE	Α	201	52.880	14.395	18.636	1.00	20.03	A
	ATOM	1076	CD1	ILE	Α	201	52.408	13.258	17.745	1.00	22.75	A
	ATOM	1077	С	ILE	Α	201	51.193	17.425	20.270	1.00	19.87	A
45	ATOM	1078	0	ILE	Α	201	50.121	17.161	20.817	1.00	20.08	A
	ATOM	1079	N	ILE	Α	202	51.508	18.633	19.815	1.00	19.94	A
	ATOM	1080	CA	ILE	Α	202	50.601	19.772	19.891	1.00	20.45	A
	ATOM	1081	СВ	ILE	Α	202	51.352	21.040	20.356	1.00	22.21	A
	ATOM	1082		ILE			50.381	22.220	20.470		22.67	A
50	ATOM	1083		ILE			52.033	20.775	21.700		24.19	A
	ATOM	1084		ILE			52.914	21.920	22.169		25.39	A
	ATOM	1085	С	ILE			50.105	19.999	18.464		20.71	А
	MOTA	1086	0	ILE			50.910	20.067	17.538		19.48	A
	ATOM	1087	N	HIS			48.795	20.108	18.270		18.65	A
55	ATOM	1088	CA	HIS			48.280	20.319	16.919		18.02	A
	ATOM	1089	СВ	HIS			46.775	20.057	16.874		16.31	A
	ATOM	1090	CG	HIS			46.199	20.136	15.495		18.36	A
	ATOM	1091		HIS			46.043	21.186	14.655		16.42	A
	ATOM	1092	ирт	HIS	А	203	45.759	19.026	14.806	T.00	19.50	A

	ATOM	1093	CE1	HIS	Α	203	45.359	19.389	13.600	1.00	17.64	A
	ATOM	1094	ME 2	HIS	7	203	45.522	20.694	13.483	1.00	20 87	A
	ATOM	1095	С	HIS			48.589	21.738	16.405	1.00		A
	ATOM	1096	0	HIS	Α	203	49.073	21.906	15.282	1.00	16.21	A
5	ATOM	1097	N	ARG	Z \	204	48.301	22.744	17.232	1.00	18 60	A
5												
	ATOM	1098	CA	ARG			48.552	24.157	16.914	1.00		A
	ATOM	1099	СВ	ARG	Α	204	49.998	24.365	16.458	1.00	21.61	А
	ATOM	1100	CG	ARG	Α	204	51.024	24.137	17.550	1.00	23.82	A
	ATOM	1101	CD	ARG			52.323	24.870	17.252	1.00		А
10												
10	ATOM	1102	NE	ARG			52.932	24.449	15.994	1.00		А
	ATOM	1103	CZ	ARG	Α	204	54.125	24.861	15.572	1.00	33.10	A
	ATOM	1104	NH1	ARG	Α	204	54.835	25.706	16.311	1.00	32.12	Α
	ATOM	1105		ARG			54.614	24.426	14.418	1.00		A
	ATOM	1106	С	ARG	Α	204	47.624	24.830	15.905	1.00		Α
15	ATOM	1107	0	ARG	Α	204	47.711	26.038	15.698	1.00	20.88	A
	ATOM	1108	N	ASP	Ά	205	46.755	24.071	15.255	1.00	18.96	Α
		1109		ASP			45.828	24.692	14.325	1.00		A
	ATOM		CA									
	ATOM	1110	СВ	ASP	Α	205	46.418	24.741	12.914	1.00	18.95	Α
	ATOM	1111	CG	ASP	Α	205	45.655	25.688	12.008	1.00	20.36	A
20	ATOM	1112	OD 1	ASP	Δ	205	44.939	26.560	12.545	1.00	20.35	Α
20												
	ATOM	1113		ASP			45.772	25.573	10.771	1.00		A
	MOTA	1114	С	ASP	Α	205	44.500	23.956	14.328	1.00	19.60	Α
	MOTA	1115	0	ASP	Α	205	43.876	23.751	13.287	1.00	21.53	Α
	ATOM	1116	N	LEU			44.063	23.569	15.521	1.00		А
25												
25	ATOM	1117	CA	LEU			42.813	22.851	15.667	1.00		A
	ATOM	1118	СВ	LEU	Α	206	42.693	22.295	17.087	1.00	18.94	A
	ATOM	1119	CG	LEU	Α	206	41.511	21.358	17.346	1.00	23.10	Α
	ATOM	1120		LEU			41.615	20.142	16.436	1.00		A
	ATOM	1121	CD2	LEU			41.504	20.933	18.808	1.00		Α
30	ATOM	1122	С	LEU	Α	206	41.639	23.772	15.361	1.00	19.05	A
	ATOM	1123	0	LEU	Α	206	41.556	24.880	15.886	1.00	19.25	Α
		1124		LYS			40.740	23.307		1.00		
	ATOM		N						14.500			A
	ATOM	1125	CA	LYS	Α	207	39.564	24.081	14.110	1.00	18.60	Α
	ATOM	1126	СВ	LYS	Α	207	39.980	25.248	13.196	1.00	18.98	A
35	ATOM	1127	CG	LYS	Δ	207	40.786	24.817	11.982	1.00	18 20	А
		1128										
	ATOM		CD	LYS			41.246	26.000	11.139	1.00		A
	MOTA	1129	CE	LYS	Α	207	42.223	25.537	10.062	1.00	23.21	Α
	ATOM	1130	NZ	LYS	Α	207	42.561	26.604	9.084	1.00	29.61	A
	ATOM	1131	С	LYS	Δ	207	38.566	23.181	13.388	1.00		A
40		1132		LYS			38.921	22.100		1.00		A
40	ATOM		0						12.915			
	ATOM	1133	N	PRO	Α	208	37.298	23.614	13.293	1.00	20.26	Α
	ATOM	1134	CD	PRO	Α	208	36.713	24.833	13.882	1.00	18.79	A
	ATOM	1135	CA	PRO	Δ	208	36.272	22.814	12.616	1.00	19.67	A
				PRO					12.608			
	ATOM	1136	СВ				35.063	23.742		1.00		A
45	MOTA	1137	CG	PRO	Α	208	35.231	24.509	13.891	1.00	21.81	Α
	ATOM	1138	С	PRO	Α	208	36.674	22.372	11.209	1.00	21.04	A
	ATOM	1139	0	PRO			36.264	21.307	10.751	1.00		Α
	ATOM	1140	N	GLU			37.474	23.188	10.528	1.00		Α
	MOTA	1141	CA	GLU	Α	209	37.928	22.872	9.170	1.00	22.64	Α
50	ATOM	1142	СВ	GLU	Α	209	38.644	24.084	8.558	1.00	23.65	Α
	ATOM	1143	CG	GLU	Δ	209	39.253	23.825	7.185	1.00	27 24	Α
	ATOM	1144	CD	GLU			40.155	24.958	6.716	1.00		A
	MOTA	1145	OE1	GLU	Α	209	39.660	26.094	6.553	1.00	29.68	Α
	MOTA	1146	OE2	GLU	Α	209	41.363	24.711	6.511	1.00	30.07	Α
55	ATOM	1147	С	GLU			38.879	21.668	9.159	1.00		А
55												
	ATOM	1148	0	GLU			38.955	20.933	8.170	1.00		A
	ATOM	1149	N	ASN	Α	210	39.600	21.490	10.263	1.00	19.90	Α
	MOTA	1150	CA	ASN	Α	210	40.574	20.412	10.436	1.00	19.44	Α
	ATOM	1151	СВ	ASN			41.744	20.912	11.287	1.00		А
	211 01.1	TT 0 T	010	7 70 11	7.7	210	· T • / I I	-0.714	-1.201	1.00	20.07	Γ

	ATOM	1152	CG	ASN	Α	210	42.746	21.698	10.479	1.00	25.77	A
	ATOM	1153		ASN			43.571	22.427	11.029	1.00		A
	ATOM	1154		ASN			42.687	21.548	9.158	1.00		A
	ATOM	1155	С	ASN			40.005	19.151	11.078	1.00		A
5	ATOM	1156	0			210	40.712	18.154	11.234	1.00		A
_	ATOM	1157	N			211	38.739	19.202	11.469	1.00		A
	ATOM	1158	CA			211	38.090	18.058	12.085	1.00		A
	ATOM	1159	СВ			211	37.336	18.488	13.354	1.00		A
	ATOM	1160		ILE			36.582	17.311	13.950	1.00		A
10	ATOM	1161		ILE			38.342	19.046	14.365	1.00		A
10	ATOM	1162		ILE			37.720	19.669	15.590	1.00		A
	ATOM	1163	C			211	37.131	17.485	11.059	1.00		A
	ATOM	1164	0			211	35.995	17.103	10.926	1.00		A
	ATOM	1165	N			212	37.599	16.486	10.317	1.00		A
15	ATOM	1166	CA	LEU			36.784	15.875	9.274	1.00		A
13	ATOM	1167	CB	LEU			37.685	15.249	8.202	1.00		A
	ATOM	1168	CG			212	38.785	16.157	7.640	1.00		A
	ATOM	1169		LEU			39.476	15.450	6.485	1.00		A
	ATOM	1170		LEU			38.188	17.482	7.166	1.00		A
20	ATOM	1171	CDZ			212	35.843	14.825	9.837	1.00		A
20	ATOM	1172	0			212	35.957	14.433	11.002	1.00		A
	ATOM	1173	N			213	34.915	14.368	9.000	1.00		A
	ATOM	1174	CA			213	33.942	13.362	9.403	1.00		A
	ATOM	1175	CB			213	32.556	14.004	9.403	1.00		A
25	ATOM	1176	CG			213	32.396	15.059	10.583	1.00		A
23	ATOM	1177		LEU			31.124	15.837	10.367	1.00		A
	ATOM	1178		LEU			32.379	14.378	11.940	1.00		
		1178								1.00		A
	ATOM		C			213	33.914	12.187	8.426			A
20	ATOM	1180	0			213	33.743	12.379	7.218	1.00		A
30	MOTA	1181	N	ASN			34.088	10.970	8.935	1.00		A
	ATOM	1182	CA	ASN			34.055	9.814	8.049	1.00		A
	ATOM	1183	CB	ASN			34.745	8.596	8.674	1.00		A
	ATOM	1184	CG	ASN			34.077	8.127	9.948	1.00		A
25	ATOM	1185		ASN			32.908	8.422	10.206	1.00		A
35	ATOM	1186		ASN			34.818	7.369	10.752	1.00		A
	ATOM	1187	C	ASN			32.618	9.466	7.693	1.00		A
	ATOM	1188	0	ASN			31.672	10.113	8.150	1.00		A
	ATOM	1189	N			215	32.459	8.433	6.879	1.00		A
40	ATOM	1190	CA			215	31.138	8.003	6.445	1.00		A
40	ATOM	1191	СВ			215	31.275	6.796	5.513	1.00		A
	ATOM	1192	CG			215	29.970	6.334	4.896	1.00		A
	ATOM	1193	CD			215	30.182	5.312	3.795	1.00		A
	ATOM	1194		GLU			30.817	4.268	4.065	1.00		A
4.5	ATOM	1195		GLU			29.716	5.556	2.660	1.00		A
45	ATOM	1196	С			215	30.188	7.673	7.601	1.00		A
	ATOM	1197	0			215	28.971	7.769	7.447	1.00		A
	ATOM	1198	N			216	30.737	7.287	8.752	1.00		A
	ATOM	1199	CA	ASP			29.914	6.953	9.917	1.00		A
- 0	ATOM	1200	СВ	ASP			30.538	5.795	10.696	1.00		А
50	ATOM	1201	CG	ASP			30.390	4.466	9.979	1.00		А
	ATOM	1202		ASP			29.274	4.170	9.499	1.00		A
	ATOM	1203		ASP			31.382	3.710	9.902	1.00		А
	MOTA	1204	С	ASP			29.697	8.135	10.862	1.00		A
	ATOM	1205	0	ASP			29.136	7.984	11.950	1.00		А
55	ATOM	1206	N	MET			30.156	9.306	10.441	1.00		A
	ATOM	1207	CA	MET			30.015	10.527	11.218	1.00		A
	ATOM	1208	СВ	MET			28.537	10.789	11.517	1.00		A
	ATOM	1209	CG	MET			27.742	11.186	10.274	1.00		A
	ATOM	1210	SD	MET	Α	217	28.464	12.616	9.430	1.00	27.57	A

	MOTA	1211	CE	MET A	. 217	27.6	79 13	3.974	10.332	1.00	26.68	A
	MOTA	1212	С	MET A	217	30.8	44 10	.618	12.502	1.00	21.51	A
	ATOM	1213	0	MET A	217	30.4	74 11	.323	13.440	1 00	18.62	А
						31.9		892			20.10	
_	ATOM	1214	N	HIS A					12.544			A
5	MOTA	1215	$^{\rm CA}$	HIS A		32.8	73 9	9.964	13.678	1.00	19.86	A
	MOTA	1216	CB	HIS A	218	33.4	82 8	3.594	13.977	1.00	20.21	A
	ATOM	1217	CG	HIS A	218	32.5	51 7	.667	14.698	1.00	22.40	A
	ATOM	1218		HIS A		31.9		5.547	14.287		21.27	А
1.0	ATOM	1219		HIS A		32.1		.863	16.011		19.59	A
10	ATOM	1220		HIS A		31.3		5.902	16.379		21.88	A
	MOTA	1221	NE2	HIS A	218	31.1	68 6	5.091	15.351	1.00	22.08	A
	ATOM	1222	С	HIS A	218	33.9	47 10	.921	13.172	1.00	19.10	A
	ATOM	1223	0	HIS A	218	34.1		.004	11.965	1.00	20.31	А
	ATOM	1224	N	ILE A		34.6		.638	14.067		17.21	A
1.5												
15	ATOM	1225	CA	ILE A		35.6		2.586	13.618		15.26	А
	MOTA	1226	СВ	ILE A	. 219	35.9	87 13	3.614	14.716	1.00	15.38	A
	MOTA	1227	CG2	ILE A	219	34.7	22 14	1.305	15.221	1.00	14.58	A
	ATOM	1228	CG1	ILE A	219	36.7	34 12	2.919	15.864	1.00	14.46	A
	ATOM	1229		ILE A		37.2		3.885	16.911		13.74	А
20	ATOM	1230	C	ILE A							16.21	
20						36.9		. 944	13.161			A
	ATOM	1231	0	ILE A		37.2		.799	13.500		15.88	A
	MOTA	1232	N	GLN A	. 220	37.6	77 12	2.711	12.378	1.00	15.62	A
	ATOM	1233	CA	GLN A	. 220	38.9	80 12	2.316	11.876	1.00	17.84	A
	ATOM	1234	СВ	GLN A	220	38.8	72 11	.595	10.525	1.00	20.00	A
25	ATOM	1235	CG	GLN A		38.4		129	10.659		26.97	A
23								343	9.372		29.95	
	ATOM	1236	CD	GLN A		38.6						A
	ATOM	1237		GLN A		37.9		.590	8.373	1.00	33.12	A
	ATOM	1238	NE2	GLN A	. 220	39.5	78 8	3.393	9.389	1.00	30.47	A
	ATOM	1239	С	GLN A	220	39.7	57 13	3.610	11.735	1.00	17.00	A
30	ATOM	1240	0	GLN A	220	39.6	0.9 1.4	1.339	10.751	1.00	18.27	А
-	ATOM	1241	N	ILE A		40.5		3.906	12.746		14.34	A
	ATOM	1242	CA	ILE A		41.3		5.120	12.753		14.46	A
	ATOM	1243	СВ	ILE A		41.8		5.416	14.175	1.00	12.30	A
	MOTA	1244	CG2	ILE A	. 221	42.7	64 16	5.656	14.167	1.00	14.78	A
35	ATOM	1245	CG1	ILE A	. 221	40.6	60 15	6.613	15.102	1.00	13.92	A
	ATOM	1246	CD1	ILE A	221	41.0	03 15	5.901	16.543	1.00	15.06	А
	ATOM	1247	C	ILE A		42.5		1.996	11.783		15.44	A
				ILE A					11.613		13.93	
	ATOM	1248	0			43.1		3.915				A
	ATOM	1249	N	THR A		42.8		5.101	11.127		15.36	A
40	MOTA	1250	CA	THR A	. 222	43.9	80 16	5.098	10.174	1.00	17.52	A
	MOTA	1251	СВ	THR A	. 222	43.4	70 15	.836	8.750	1.00	19.92	A
	ATOM	1252	OG1	THR A	222	44.5	87 15	6.637	7.875	1.00	18.78	А
	ATOM	1253		THR A		42.6		.018	8.257		18.16	А
	ATOM	1254	C	THR A		44.7		.428	10.192		19.60	A
15												
45	ATOM	1255	0	THR A		44.5		3.257	11.084		18.59	А
	MOTA	1256	N	ASP A	. 223	45.6	30 17	.610	9.216	1.00	18.69	A
	MOTA	1257	CA	ASP A	. 223	46.4	40 18	8.825	9.069	1.00	20.12	A
	ATOM	1258	СВ	ASP A	223	45.5	32 20	0.065	9.108	1.00	23.51	А
	ATOM	1259	CG	ASP A		46.2		.335	8.670		27.09	А
50									7.975		26.28	
50	ATOM	1260		ASP A		47.2		.227				A
	ATOM	1261		ASP A		45.7		2.438	9.009		26.15	A
	MOTA	1262	С	ASP A	. 223	47.5	16 18	3.913	10.150	1.00	21.73	A
	ATOM	1263	0	ASP A	223	47.4	39 19	3.751	11.055	1.00	22.76	A
	ATOM	1264	N	PHE A		48.5		3.063	10.027		20.75	А
55	ATOM	1265	CA	PHE A		49.6		.988	11.009		20.11	A
55												
	ATOM	1266	СВ	PHE A		49.8		5.527	11.424		20.62	A
	ATOM	1267	CG	PHE A		48.6		5.991	12.263		21.41	A
	ATOM	1268	CD1	PHE A	224	48.5	98 16	5.312	13.614	1.00	23.05	A
	ATOM	1269		PHE A		47.6	81 15	5.212	11.693		22.27	А
	-	-	_		-			_				

	ATOM	1270	CE1	PHE	Α	224	47.528	15.868	14.389	1.00	23.30	А
	ATOM	1271	CE2	PHE	Α	224	46.606	14.763	12.457		21.11	А
	ATOM	1272	CZ	PHE	Α	224	46.530	15.093	13.807	1.00	22.02	А
	ATOM	1273	С	PHE	Α	224	50.957	18.583	10.619	1.00	20.45	А
5	ATOM	1274	0	PHE			51.905	18.547	11.407		20.73	А
	ATOM	1275	N	GLY	Α	225	51.049	19.125	9.412	1.00	22.02	А
	ATOM	1276	CA	GLY	А	225	52.301	19.713	8.981		22.66	А
	ATOM	1277	С	GLY			52.742	20.822	9.920	1.00	24.99	А
	ATOM	1278	0	GLY	Α	225	53.939	21.041	10.122	1.00	24.52	А
10	ATOM	1279	N	THR	Α	226	51.779	21.524	10.508	1.00	23.50	А
	ATOM	1280	CA	THR	Α	226	52.106	22.613	11.416	1.00	25.16	А
	ATOM	1281	СВ	THR	А	226	51.199	23.829	11.160		24.76	А
	ATOM	1282	OG1	THR			49.831	23.410	11.113		22.68	А
	ATOM	1283	CG2	THR	А	226	51.571	24.490	9.834		25.00	А
15	ATOM	1284	С	THR	Α	226	52.046	22.233	12.894		25.79	А
	ATOM	1285	0	THR	Α	226	52.019	23.100	13.768		24.54	А
	ATOM	1286	N	ALA	А	227	52.037	20.935	13.173	1.00	24.97	А
	ATOM	1287	CA	ALA	Α	227	52.004	20.475	14.550		25.49	А
	ATOM	1288	СВ	ALA	А	227	51.659	18.993	14.607	1.00	22.85	А
20	ATOM	1289	С	ALA	А	227	53.384	20.715	15.149		27.70	А
	ATOM	1290	0	ALA	Α	227	54.331	21.047	14.435	1.00	26.60	A
	ATOM	1291	N	LYS			53.491	20.558	16.461		28.53	А
	ATOM	1292	CA	LYS	А	228	54.760	20.745	17.149	1.00	32.12	А
	ATOM	1293	СВ	LYS	А	228	54.699	21.974	18.054		33.81	А
25	ATOM	1294	CG	LYS			56.007	22.294	18.765		41.23	А
	ATOM	1295	CD	LYS	Α	228	57.082	22.725	17.768	1.00	47.57	A
	ATOM	1296	CE	LYS	А	228	58.401	23.056	18.462	1.00	49.82	А
	ATOM	1297	NΖ	LYS	Α	228	59.459	23.425	17.480	1.00	51.49	A
	ATOM	1298	С	LYS	Α	228	55.019	19.504	17.985	1.00	33.25	А
30	ATOM	1299	0	LYS			54.190	19.129	18.815		33.70	А
	ATOM	1300	N	VAL			56.159	18.860	17.756		33.64	A
	ATOM	1301	CA	VAL			56.516	17.661	18.501	1.00	34.66	A
	ATOM	1302	СВ	VAL			57.248	16.646	17.609		33.50	А
	ATOM	1303		VAL			57.619	15.419	18.415		32.34	А
35	ATOM	1304	CG2	VAL	Α	229	56.370	16.264	16.436	1.00	34.25	A
	ATOM	1305	С	VAL	Α	229	57.420	18.035	19.668	1.00	37.57	А
	ATOM	1306	0	VAL	А	229	58.581	18.392	19.474	1.00	35.91	А
	ATOM	1307	N	LEU			56.877	17.948	20.878	1.00	40.57	А
	ATOM	1308	CA	LEU	Α	230	57.615	18.289	22.088	1.00	46.10	А
40	ATOM	1309	СВ	LEU			56.654	18.417	23.270	1.00	44.71	А
	ATOM	1310	CG	LEU	Α	230	55.627	19.545	23.207	1.00	44.50	А
	ATOM	1311	CD1	LEU	Α	230	54.673	19.430	24.383	1.00	44.39	A
	ATOM	1312	CD2	LEU	Α	230	56.340	20.885	23.214	1.00	44.81	А
	ATOM	1313	С	LEU			58.695	17.279	22.440	1.00	50.42	А
45	ATOM	1314	0			230	58.603	16.104	22.089		51.64	А
	ATOM	1315	N			231	59.717	17.756	23.145	1.00	55.81	А
	ATOM	1316	CA	SER	Α	231	60.824	16.914	23.583		61.14	A
	ATOM	1317	СВ			231	62.077	17.200	22.750		61.27	A
	ATOM	1318	OG			231	62.444	18.568	22.823	1.00	62.85	А
50	ATOM	1319	С	SER			61.124	17.126	25.071	1.00	64.65	А
	ATOM	1320	0	SER	Α	231	61.392	16.164	25.794		65.70	А
	ATOM	1321	N	PRO			61.081	18.387	25.549		67.54	А
	ATOM	1322	CD	PRO			60.854	19.651	24.823	1.00	68.60	А
	ATOM	1323	CA	PRO			61.358	18.655	26.966		68.74	A
55	ATOM	1324	СВ	PRO			61.109	20.158	27.086		68.83	A
	ATOM	1325	CG	PRO			61.505	20.666	25.737		68.96	A
	ATOM	1326	С	PRO			60.460	17.846	27.899		69.17	A
	ATOM	1327	0	PRO			59.335	17.494	27.541		69.94	A
	ATOM	1328	N	ALA			57.424	23.198	27.637		80.06	A

	ATOM	1329	CA	ALA	Α	237	56.783	23.047	26.335	1.00	79.29	A
	ATOM	1330	СВ	ALA			55.275	22.907	26.512	1 00	78.64	А
	ATOM	1331	С	ALA	Α	237	57.092	24.239	25.433	1.00	79.07	A
	ATOM	1332	0	ALA	Α	237	56.250	25.113	25.249	1.00	79.47	A
5	ATOM	1333	N	ALA			58.297	24.280	24.871	1 00	78.57	A
,												
	ATOM	1334	CA	ALA			58.683	25.383	23.992		78.50	A
	ATOM	1335	СВ	ALA	Α	238	60.186	25.347	23.728	1.00	78.50	A
	ATOM	1336	С	ALA	Α	238	57.920	25.327	22.673	1.00	78.15	A
	ATOM	1337	0	ALA			57.243	24.341	22.375		77.96	A
10												
10	ATOM	1338	N	ALA			58.027	26.393	21.887		77.28	А
	ATOM	1339	CA	ALA	Α	239	57.338	26.452	20.603	1.00	76.27	A
	ATOM	1340	СВ	ALA	Α	239	55.849	26.489	20.827	1.00	76.61	А
	ATOM	1341	C	ALA			57.766	27.667	19.793		75.38	A
	ATOM	1342	0	ALA	Α	239	58.955	27.955	19.700	1.00	75.89	A
15	ATOM	1343	N	ASN	Α	240	56.781	28.357	19.214	1.00	73.95	A
	ATOM	1344	CA	ASN	А	240	56.967	29.553	18.389	1.00	71.07	A
		1345		ASN			58.151	30.400	18.874		71.47	A
	ATOM		СВ									
	ATOM	1346	CG	ASN	Α	240	59.459	30.055	18.174		72.06	Α
	ATOM	1347	OD1	ASN	Α	240	59.575	30.149	16.943	1.00	72.03	A
20	ATOM	1348	ND2	ASN	Δ	240	60.470	29.665	18.964	1.00	71.91	А
20												
	ATOM	1349	С	ASN			57.188	29.178	16.928		69.41	A
	ATOM	1350	0	ASN	Α	240	57.480	28.024	16.624		70.09	A
	ATOM	1351	N	ALA	Α	241	57.055	30.165	16.038	1.00	66.62	A
	ATOM	1352	CA	ALA			57.246	30.013	14.585		63.94	A
25												
25	ATOM	1353	С	ALA			55.952	30.080	13.772		60.63	A
	ATOM	1354	0	ALA	Α	241	55.840	30.880	12.845	1.00	61.29	A
	ATOM	1355	СВ	ALA	Α	241	57.979	28.704	14.246	1.00	65.23	A
	ATOM	1356	N	PHE			54.984	29.236	14.113		56.72	А
	ATOM	1357	CA	PHE			53.712	29.196	13.394		52.53	А
30	ATOM	1358	СВ	PHE	Α	242	53.419	27.767	12.923	1.00	49.14	A
	ATOM	1359	CG	PHE	Α	242	52.040	27.590	12.354	1.00	47.38	A
		1360		PHE			51.731	28.067	11.085		47.69	
	ATOM											A
	ATOM	1361	CD2	PHE	А	242	51.038	26.975	13.102	1.00	45.45	A
	ATOM	1362	CE1	PHE	Α	242	50.445	27.937	10.565	1.00	46.75	A
35	ATOM	1363	CE2	PHE	Ά	242	49.751	26.840	12.594	1.00	45.41	A
							49.453					
	ATOM	1364	CZ	PHE				27.323	11.322		46.55	A
	ATOM	1365	С	PHE	Α	242	52.534	29.688	14.229	1.00	50.08	A
	ATOM	1366	0	PHE	Α	242	52.502	29.505	15.444	1.00	49.86	A
	ATOM	1367	N	VAL	Ά	243	51.566	30.305	13.557		47.67	A
40		1368	CA	VAL			50.355	30.809	14.200		46.21	A
40	ATOM											
	ATOM	1369	СВ	VAL	Α	243	50.340	32.352	14.258	1.00	47.36	A
	ATOM	1370	CG1	VAL	Α	243	49.012	32.844	14.825	1.00	47.54	A
	ATOM	1371	CG2	VAL	Δ	243	51.497	32.842	15.109	1.00	48.50	A
	ATOM	1372	C	VAL			49.150	30.342	13.389		44.12	
												A
45	ATOM	1373	0	VAL	Α	243	48.956	30.765	12.247	1.00	44.46	A
	ATOM	1374	N	GLY	Α	244	48.348	29.467	13.985	1.00	40.48	A
	ATOM	1375	CA	GLY	Z \	244	47.176	28.941	13.306	1 00	37.65	А
	ATOM	1376	С	GLY			46.101	29.960	12.964		35.39	A
	ATOM	1377	0	GLY			46.313	31.168	13.065	1.00	35.92	A
50	MOTA	1378	N	THR	Α	245	44.936	29.463	12.560	1.00	33.30	A
	ATOM	1379	CA	THR			43.813	30.312	12.184	1 00	30.20	A
	ATOM	1380	СВ	THR			42.593	29.450	11.829		32.00	A
	MOTA	1381	OG1	THR	Α	245	42.952	28.573	10.755	1.00	32.81	A
	MOTA	1382	CG2	THR	Α	245	41.419	30.319	11.390	1.00	28.34	A
55	ATOM	1383	С	THR			43.476	31.296	13.296		27.96	А
55												
	ATOM	1384	0	THR			43.212	30.907	14.434		25.46	A
	ATOM	1385	N	ALA	Α	246	43.486	32.576	12.938	1.00	25.22	A
	MOTA	1386	CA	ALA	Α	246	43.247	33.675	13.867	1.00	23.27	A
	ATOM	1387	СВ	ALA			42.956	34.955	13.082		22.94	А
	211 01.1	±001	010	11117	17	210	12.550	51.555	10.002	 00	,	1-1

	ATOM	1388	С	ALA	Δ	246	42.178	33.475	14.934	1.00	21.27	А
	ATOM	1389	0	ALA			42.431	33.705	16.114		20.93	A
	ATOM	1390	N			247	40.988	33.047	14.536		19.67	A
	ATOM	1391	CA	GLN			39.911	32.886	15.504		20.17	A
5	ATOM	1391		GLN			38.608		14.779		21.89	
3		1392	CB					32.535				A
	ATOM		CG			247	38.522	33.076	13.355		26.18	A
	ATOM	1394	CD			247	37.220	33.794	13.064		27.30	A
	ATOM	1395		GLN			36.172	33.447	13.605		30.13	A
1.0	ATOM	1396		GLN			37.278	34.792	12.189		28.70	A
10	ATOM	1397	С	GLN			40.181	31.849	16.595		19.43	A -
	ATOM	1398	0			247	39.546	31.883	17.648		18.93	A
	ATOM	1399	N	TYR			41.132	30.948	16.359		18.60	A
	ATOM	1400	CA	TYR			41.441	29.896	17.329		19.20	A
	ATOM	1401	СВ	TYR			41.333	28.529	16.642		17.53	А
15	ATOM	1402	CG	TYR			40.013	28.362	15.927		19.32	A
	ATOM	1403	CD1	TYR	Α	248	38.859	28.010	16.625	1.00	17.69	A
	ATOM	1404	CE1	TYR	Α	248	37.617	27.976	15.990	1.00	18.18	A
	ATOM	1405	CD2	TYR	Α	248	39.897	28.664	14.569	1.00	16.87	A
	ATOM	1406	CE2	TYR	Α	248	38.665	28.635	13.924	1.00	19.17	A
20	ATOM	1407	CZ	TYR	Α	248	37.527	28.295	14.643	1.00	19.46	A
	ATOM	1408	OH	TYR	Α	248	36.299	28.311	14.023	1.00	18.98	A
	ATOM	1409	С	TYR	Α	248	42.810	30.039	17.993	1.00	20.42	А
	ATOM	1410	0	TYR	Α	248	43.208	29.191	18.792	1.00	19.19	А
	ATOM	1411	N	VAL	Α	249	43.523	31.114	17.673	1.00	20.20	А
25	ATOM	1412	CA	VAL			44.841	31.343	18.251		20.91	А
	ATOM	1413	СВ	VAL			45.542	32.532	17.570		21.18	A
	ATOM	1414		VAL			46.821	32.896	18.317		22.45	A
	ATOM	1415		VAL			45.862	32.170	16.139		24.01	A
	ATOM	1416	C			249	44.764	31.606	19.750		21.52	A
30	ATOM	1417	0	VAL			43.915	32.368	20.216		22.72	A
30	ATOM	1418	N			250	45.654	30.965	20.503		20.70	A
	ATOM	1419	CA			250	45.697	31.133	21.951		21.65	A
	ATOM	1419	CB			250	46.370	29.919	22.613		22.02	A
	ATOM	1420	OG			250	47.692	29.725	22.132		22.12	A
25												
35	ATOM	1422	C			250	46.476	32.402	22.280		22.13	A
	ATOM	1423	0			250	47.332	32.828	21.511		22.77	A
	ATOM	1424	N			251	46.180	33.029	23.425		22.23	A
	ATOM	1425	CD			251	45.163	32.684	24.433		22.97	A
40	ATOM	1426	CA			251	46.893	34.254	23.800		22.52	A
40	ATOM	1427	СВ			251	46.233	34.650	25.127		23.06	A
	ATOM	1428	CG			251	45.726	33.329	25.676		22.55	A
	ATOM	1429	С			251	48.414	34.115	23.907		22.15	A
	ATOM	1430	0			251	49.143	35.047	23.563		22.62	A
	ATOM	1431	N	GLU			48.901	32.966	24.367		20.69	A
45	ATOM	1432	CA	GLU			50.347	32.772	24.500		21.40	A
	MOTA	1433	СВ	GLU			50.673	31.382	25.071		20.59	A
	MOTA	1434	CG	GLU			49.993	30.232	24.352	1.00	21.91	A
	MOTA	1435	CD	GLU	Α	252	48.691	29.822	25.014	1.00	21.51	A
	MOTA	1436	OE1	GLU	Α	252	47.989	30.707	25.550	1.00	21.46	A
50	ATOM	1437	OE2	GLU	Α	252	48.367	28.613	24.993	1.00	20.23	A
	ATOM	1438	С	GLU	Α	252	51.071	32.970	23.167	1.00	22.99	A
	ATOM	1439	0	GLU	Α	252	52.191	33.480	23.136	1.00	23.17	A
	ATOM	1440	N	LEU	Α	253	50.441	32.576	22.064		23.00	А
	ATOM	1441	CA	LEU			51.068	32.753	20.758		25.62	А
55	ATOM	1442	СВ	LEU	Α	253	50.277	32.029	19.669		26.75	A
	ATOM	1443	CG	LEU			50.743	30.620	19.296		31.87	А
	ATOM	1444		LEU			50.433	29.651	20.422		31.81	A
	ATOM	1445		LEU			50.044	30.179	18.015		31.86	A
	ATOM	1446	C			253	51.201	34.228	20.371		26.94	A
					_							

	ATOM	1447	0	LEU	Α	253	52.107	34.601	19.626	1.00	27.09	А
	ATOM	1448	N			254	50.297	35.059	20.877		25.83	A
	ATOM	1449	CA	LEU			50.297	36.485	20.564		27.26	А
	ATOM	1450	СВ	LEU			48.858	37.006	20.564		25.84	А
5	ATOM	1451	CG			254	47.882	36.290	19.621		24.69	A
	ATOM	1452		LEU			46.459	36.724	19.932		23.64	A
	ATOM	1453		LEU			48.236	36.597	18.177		24.24	А
	ATOM	1454	С			254	51.134	37.314	21.537		30.62	А
	ATOM	1455	0			254	51.633	38.383	21.187		32.35	А
10	ATOM	1456	N			255	51.292	36.821	22.758		32.47	А
	ATOM	1457	CA			255	52.056	37.547	23.759	1.00	36.70	А
	ATOM	1458	СВ			255	51.368	37.478	25.127		34.51	А
	ATOM	1459	OG1	THR			51.188	36.106	25.494		35.49	А
	ATOM	1460		THR			50.013	38.166	25.077		33.40	А
15	ATOM	1461	С	THR	Α	255	53.477	37.035	23.910	1.00	40.09	А
	ATOM	1462	0			255	54.430	37.793	23.772		43.69	А
	ATOM	1463	N	GLU	Α	256	53.617	35.747	24.189	1.00	44.77	А
	ATOM	1464	CA			256	54.932	35.144	24.382	1.00	49.15	А
	ATOM	1465	СВ	GLU	Α	256	54.866	34.143	25.534	1.00	51.24	А
20	ATOM	1466	CG	GLU	Α	256	54.514	34.786	26.862		56.03	А
	ATOM	1467	CD			256	54.053	33.780	27.893	1.00	58.83	А
	ATOM	1468	OE1	GLU			54.766	32.776	28.107		62.13	А
	ATOM	1469		GLU			52.979	33.996	28.494		60.34	А
	ATOM	1470	C			256	55.475	34.456	23.137		50.09	A
25	ATOM	1471	0	GLU	Α	256	56.616	33.995	23.127		50.42	А
	ATOM	1472	N			257	54.658	34.389	22.090		51.21	A
	ATOM	1473	CA	LYS	Α	257	55.064	33.746	20.845		51.22	А
	ATOM	1474	СВ			257	56.244	34.502	20.227		53.28	A
	ATOM	1475	CG	LYS			56.558	34.125	18.790		55.19	A
30	ATOM	1476	CD			257	57.709	34.961	18.253		57.52	A
	ATOM	1477	CE			257	57.952	34.694	16.777		58.52	A
	ATOM	1478	NZ			257	58.290	33.268	16.515		60.88	А
	ATOM	1479	C			257	55.467	32.302	21.138		50.74	A
	ATOM	1480	0			257	56.432	31.790	20.577		52.26	A
35	ATOM	1481	N	SER	Α	258	54.721	31.654	22.027	1.00	48.07	A
	ATOM	1482	CA			258	54.999	30.273	22.402		46.87	A
	ATOM	1483	СВ			258	55.590	30.229	23.812		48.88	А
	ATOM	1484	OG			258	54.741	30.892	24.734		53.14	A
	ATOM	1485	С			258	53.735	29.415	22.342		44.07	A
40	ATOM	1486	0			258	52.617	29.932	22.417		44.17	А
	ATOM	1487	N			259	53.917	28.105	22.204		38.30	A
	ATOM	1488	CA	ALA	Α	259	52.793	27.180	22.127	1.00	34.73	А
	ATOM	1489	СВ	ALA			52.551	26.779	20.684	1.00	34.16	A
	MOTA	1490	С			259	53.042	25.940	22.977		32.34	А
45	ATOM	1491	0			259	54.172	25.459	23.086		31.81	А
	ATOM	1492	N			260	51.975	25.428	23.579		28.58	А
	ATOM	1493	CA			260	52.056	24.244	24.425		26.27	A
	ATOM	1494	СВ			260	52.183	24.654	25.892		26.53	A
	ATOM	1495	SG			260	50.846	25.739	26.469		32.91	А
50	ATOM	1496	С	CYS	Α	260	50.786	23.435	24.224		22.83	A
	ATOM	1497	0			260	49.892	23.856	23.495		22.14	А
	ATOM	1498	N			261	50.706	22.277	24.868		20.02	A
	ATOM	1499	CA			261	49.526	21.434	24.744		20.65	А
	ATOM	1500	СВ			261	49.619	20.243	25.696		23.28	A
55	ATOM	1501	CG			261	50.716	19.253	25.347		27.44	A
	ATOM	1502	CD			261	50.732	18.117	26.350		29.98	A
	ATOM	1503	CE			261	51.922	17.203	26.134		32.34	A
	ATOM	1504	ΝZ			261	51.940	16.121	27.153		33.28	A
	ATOM	1505	C			261	48.268	22.229	25.062		19.20	A

	ATOM	1506	0	LYS	A	261	4	47.253	22.092	24.387	1.00	18.08	А
	ATOM	1507	N			262		48.358	23.068	26.089		16.92	А
	ATOM	1508	CA			262		47.235	23.883	26.534		18.13	А
	ATOM	1509	СВ			262		47.644	24.698	27.770		18.27	А
5	ATOM	1510	OG			262		46.517	25.258	28.421		22.53	А
	ATOM	1511	С	SER	Α	262	4	46.736	24.811	25.424	1.00	16.77	А
	ATOM	1512	0	SER	А	262	4	45.591	25.254	25.450	1.00	15.69	А
	ATOM	1513	N			263	4	47.595	25.118	24.456	1.00	16.44	А
	ATOM	1514	CA	SER	Α	263	4	47.175	25.970	23.347	1.00	16.89	А
10	ATOM	1515	СВ	SER	Α	263	4	48.340	26.228	22.382	1.00	18.49	А
	ATOM	1516	OG	SER	Α	263	4	49.402	26.909	23.031	1.00	22.10	A
	ATOM	1517	С	SER	А	263	4	46.040	25.257	22.612	1.00	17.79	А
	ATOM	1518	0	SER	Α	263	4	45.099	25.898	22.148	1.00	17.57	A
	ATOM	1519	N	ASP	Α	264	4	46.119	23.928	22.517	1.00	16.30	A
15	ATOM	1520	CA	ASP	Α	264	4	45.069	23.166	21.836	1.00	16.72	A
	ATOM	1521	СВ	ASP	Α	264	4	45.483	21.704	21.620	1.00	15.92	A
	ATOM	1522	CG	ASP	Α	264	4	16.544	21.539	20.548	1.00	17.93	A
	MOTA	1523	OD1	ASP	Α	264	4	46.642	22.412	19.661	1.00	16.78	A
	ATOM	1524	OD2	ASP	А	264	4	47.265	20.515	20.579	1.00	16.64	A
20	ATOM	1525	C	ASP	Α	264	4	43.773	23.194	22.646		17.67	A
	ATOM	1526	0	ASP	A	264	4	42.681	23.197	22.076	1.00	18.27	A
	ATOM	1527	N	LEU	Α	265	4	43.898	23.205	23.974	1.00	15.49	A
	ATOM	1528	CA	LEU	А	265	4	12.730	23.232	24.849	1.00	14.75	A
	ATOM	1529	СВ	LEU	Α	265	4	43.147	23.038	26.313	1.00	11.38	A
25	ATOM	1530	CG	LEU	Α	265	4	43.711	21.641	26.621	1.00	14.04	A
	MOTA	1531		LEU			4	44.249	21.579	28.052	1.00	13.96	A
	MOTA	1532	CD2	LEU	А	265	4	42.619	20.603	26.416		11.62	A
	MOTA	1533	С			265		41.999	24.557	24.675		15.13	A
	MOTA	1534	0			265		40.777	24.620	24.785		16.75	A
30	MOTA	1535	N	TRP	Α	266	4	42.746	25.622	24.405	1.00	16.08	A
	MOTA	1536	CA			266		42.118	26.918	24.184		16.96	A
	ATOM	1537	СВ			266	4	43.176	28.015	24.023		17.28	A
	MOTA	1538	CG			266		42.618	29.326	23.521		20.54	A
	ATOM	1539		TRP				42.313	30.490	24.301		20.07	A
35	ATOM	1540	CE2	TRP				41.782	31.459	23.417		20.46	A
	ATOM	1541	CE3					42.435	30.810	25.660		20.68	A
	ATOM	1542		TRP				42.270	29.631	22.231		19.53	A
	ATOM	1543		TRP				11.769	30.908	22.163		19.61	A
40	ATOM	1544	CZ2					41.372	32.727	23.850		20.90	A
40	ATOM	1545		TRP				42.026	32.073	26.091		19.45	A
	ATOM	1546	CH2					41.501	33.015	25.185		20.71	A
	ATOM	1547	С			266		41.284	26.795	22.913		17.22	A
	ATOM	1548	0			266		40.139	27.240	22.863		18.03	A
45	ATOM	1549	N	ALA				41.863	26.181	21.886		17.50	A
45	ATOM	1550	CA	ALA				41.155	25.990	20.626		16.16	A
	ATOM	1551	СВ	ALA				42.050	25.290	19.621		14.28	A
	ATOM	1552	C	ALA				39.901	25.159	20.891		16.28	A
	ATOM	1553	0	ALA				38.835	25.436	20.346 21.739		16.46	A
50	MOTA	1554	N			268		40.031 38.890	24.144			16.57	A
50	ATOM ATOM	1555 1556	CA CB	LEU LEU				39.292	23.299 22.260	22.084		17.03 15.35	A
		1557	CG						21.429	23.139 23.754			A
	ATOM	1558		LEU LEU				38.158	20.578			19.00 16.17	A
	ATOM ATOM	1559		LEU				37.505 38.718	20.578	22.678 24.881		17.49	A A
55	ATOM	1560	CD2	LEU				37.766	24.179	22.628		15.72	A A
55	ATOM	1561	0	LEU				36.603	24.179	22.247		15.72	A
	ATOM	1562	N	GLY				38.119	25.099	23.520		14.34	A
	ATOM	1563	CA			269		37.124	25.989	24.092		13.39	A
	ATOM	1564	C			269		36.406	26.808	23.031		14.94	A
	AT ON	T004	$\overline{}$	ОПІ	17	200		00.400	20.000	20.UJI	1. 00	11.JT	A

	ATOM	1565	0	GLY	Α	269	35.193	27.014	23.114	1.00 14.76	А
	ATOM	1566	N	CYS	Α	270	37.146	27.279	22.030	1.00 13.86	А
	ATOM	1567	CA	CYS	A	270	36.539	28.061	20.958	1.00 16.80	A
	ATOM	1568	СВ	CYS	Α	270	37.611	28.634	20.023	1.00 15.97	A
5	ATOM	1569	SG	CYS	A	270	38.751	29.810	20.780	1.00 20.48	A
	MOTA	1570	С	CYS	Α	270	35.598	27.175	20.140	1.00 17.50	A
	MOTA	1571	0	CYS	Α	270	34.516	27.604	19.741	1.00 18.38	A
	ATOM	1572	N	ILE	Α	271	36.022	25.939	19.887	1.00 16.99	A
	MOTA	1573	CA	ILE	Α	271	35.221	25.004	19.104	1.00 16.66	A
10	ATOM	1574	СВ	ILE	Α	271	36.038	23.741	18.778	1.00 16.53	A
	MOTA	1575	CG2	ILE	Α	271	35.155	22.694	18.102	1.00 16.34	A
	MOTA	1576	CG1	ILE	Α	271	37.222	24.129	17.882	1.00 15.59	A
	MOTA	1577	CD1	ILE	Α	271	38.239	23.018	17.690	1.00 14.88	A
	ATOM	1578	С	ILE	Α	271	33.920	24.626	19.809	1.00 16.74	A
15	ATOM	1579	0	ILE	Α	271	32.865	24.576	19.179	1.00 17.12	A
	ATOM	1580	N	ILE	Α	272	33.990	24.357	21.111	1.00 16.13	A
	ATOM	1581	CA	ILE	Α	272	32.785	24.021	21.862	1.00 18.30	A
	ATOM	1582	СВ	ILE	Α	272	33.097	23.747	23.346	1.00 17.77	A
	ATOM	1583	CG2	ILE	Α	272	31.796	23.666	24.152	1.00 17.96	A
20	MOTA	1584		ILE			33.877	22.437	23.481	1.00 19.55	A
	ATOM	1585	CD1	ILE	Α	272	34.446	22.217	24.886	1.00 18.64	A
	MOTA	1586	С			272	31.824	25.207	21.776	1.00 19.51	A
	MOTA	1587	0			272	30.624	25.037	21.554	1.00 20.44	A
	MOTA	1588	N	TYR			32.362	26.409	21.947	1.00 18.52	A
25	ATOM	1589	CA	TYR			31.553	27.615	21.881	1.00 20.48	A
	ATOM	1590	СВ	TYR			32.418	28.847	22.162	1.00 18.98	A
	ATOM	1591	CG			273	31.663	30.161	22.125	1.00 20.26	A
	ATOM	1592		TYR			31.229	30.709	20.916	1.00 20.67	A
	ATOM	1593		TYR			30.536	31.917	20.880	1.00 20.98	A
30	ATOM	1594		TYR			31.383	30.857	23.302	1.00 19.82	A
	ATOM	1595	CE2	TYR			30.691	32.062	23.280	1.00 20.62	A
	ATOM	1596	CZ	TYR			30.271	32.587	22.067	1.00 21.15	A
	ATOM	1597	OH	TYR			29.588	33.776	22.049	1.00 21.86	A
	ATOM	1598	С			273	30.902	27.730	20.507	1.00 21.54	A
35	ATOM	1599	0	TYR			29.719	28.049	20.401	1.00 22.80	A
	ATOM	1600	N	GLN			31.676	27.454	19.461	1.00 21.05	A
	ATOM	1601	CA			274	31.176	27.538	18.095	1.00 21.48	A
	ATOM	1602	СВ			274	32.323	27.341	17.097	1.00 21.41	A
40	ATOM	1603	CG	GLN			31.934	27.596	15.645	1.00 23.15	A
40	ATOM	1604	CD	GLN			33.131	27.588	14.706	1.00 24.80	A
	ATOM	1605		GLN			34.276	27.446	15.139	1.00 22.51	A
	ATOM	1606	NE2				32.870	27.750	13.413	1.00 22.96	A
	ATOM	1607	C	GLN			30.076	26.517	17.828	1.00 21.51	A
45	ATOM	1608	0	GLN			29.123	26.806	17.108	1.00 20.50	A
45	ATOM	1609	N			275	30.207	25.324	18.403	1.00 21.44	A
	ATOM	1610	CA			275	29.196	24.282	18.208	1.00 20.95	A
	ATOM	1611	CB			275	29.645	22.958	18.846	1.00 19.11	A
	ATOM	1612	CG CD1	LEU			30.775	22.182	18.159	1.00 21.43 1.00 17.64	A
50	MOTA	1613 1614		LEU LEU			31.118	20.936	18.963		A
50	MOTA	1615					30.342 27.860	21.795	16.754 18.815	1.00 20.34 1.00 21.32	A
	ATOM		C	LEU				24.697 24.461	18.229	1.00 21.32	A
	ATOM	1616 1617	O N	LEU			26.802	25.322	19.987	1.00 19.75	A
	ATOM ATOM	1618	n CA	VAL VAL			27.921 26.724	25.750	20.702	1.00 19.10	A A
55		1619	CB	VAL				25.730	20.702	1.00 22.47	
55	ATOM ATOM	1620		VAL			27.011 25.742	26.291	22.217	1.00 20.87	A A
	ATOM	1621		VAL			27.550	24.558	22.766	1.00 19.88	A
	ATOM	1622	C			276	26.127	27.075	20.211	1.00 19.43	A
	ATOM	1623	0			276	24.910	27.199	20.211	1.00 23.09	A
	AT ON	T070	\circ	٧ДП	17	210	2 T . J I U	∠ 1 • ± ∋ Э	20.070	1.00 Z1.30	A

	MOTA	1624	N	ALA A 2	77	26.983	28.062	19.965	1.00	24.56	A
	ATOM	1625	CA	ALA A 2	77	26.533	29.374	19.518	1.00	24.72	A
	ATOM	1626	СВ	ALA A 2		27.504	30.444	19.999		24.36	A
	MOTA	1627	С	ALA A 2		26.378	29.458	18.005		25.76	A
5	MOTA	1628	0	ALA A 2	77	25.577	30.242	17.502	1.00	26.39	A
	ATOM	1629	N	GLY A 2	78	27.142	28.651	17.280	1.00	25.13	A
	ATOM	1630	CA	GLY A 2		27.062	28.673	15.834		25.58	A
	MOTA	1631	С	GLY A 2		28.163	29.524	15.231		26.50	A
	MOTA	1632	0	GLY A 2	78	28.374	29.510	14.015	1.00	28.17	A
10	ATOM	1633	N	LEU A 2	79	28.866	30.262	16.086	1.00	24.44	A
	ATOM	1634	CA	LEU A 2		29.962	31.130	15.656		25.21	А
	ATOM	1635	СВ	LEU A 2		29.468	32.575	15.500		25.78	А
	MOTA	1636	CG	LEU A 2	79	28.364	32.899	14.490	1.00	28.17	A
	ATOM	1637	CD1	LEU A 2	79	27.922	34.344	14.684	1.00	26.60	A
15	ATOM	1638		LEU A 2		28.862	32.670	13.071		26.52	A
13											
	ATOM	1639	С	LEU A 2		31.093	31.116	16.687		23.47	A
	MOTA	1640	0	LEU A 2	79	30.848	30.994	17.882	1.00	24.44	A
	ATOM	1641	N	PRO A 2	80	32.349	31.239	16.236	1.00	23.35	A
	ATOM	1642	CD	PRO A 2		32.831	31.404	14.855		22.26	А
20											
20	ATOM	1643	CA	PRO A 2		33.464	31.239	17.189		23.81	A
	MOTA	1644	СВ	PRO A 2	80	34.692	31.293	16.282	1.00	23.24	A
	ATOM	1645	CG	PRO A 2	80	34.189	32.020	15.073	1.00	24.89	А
	ATOM	1646	С	PRO A 2		33.353	32.444	18.137	1 00	22.69	А
	ATOM	1647	0	PRO A 2		32.750	33.457	17.788		22.11	A
25	MOTA	1648	N	PRO A 2	81	33.939	32.344	19.345	1.00	23.06	A
	MOTA	1649	CD	PRO A 2	81	34.810	31.223	19.734	1.00	21.37	A
	ATOM	1650	CA	PRO A 2	81	33.935	33.375	20.395	1.00	23.67	A
	ATOM	1651		PRO A 2		34.781	32.751			24.89	
			СВ					21.509			A
	MOTA	1652	CG	PRO A 2	81	34.749	31.287	21.219	1.00	25.24	A
30	MOTA	1653	С	PRO A 2	81	34.481	34.752	20.017	1.00	23.75	A
	ATOM	1654	0	PRO A 2	81	33.869	35.781	20.317	1.00	21.02	A
	ATOM	1655	N	PHE A 2		35.644	34.763	19.379		22.17	A
	MOTA	1656	CA	PHE A 2		36.293	36.007	18.998		23.16	A
	MOTA	1657	CB	PHE A 2	82	37.765	35.943	19.406	1.00	21.01	A
35	ATOM	1658	CG	PHE A 2	82	37.975	35.482	20.822	1.00	22.66	A
	ATOM	1659	CD1			37.806	36.361	21.888		20.06	A
	ATOM	1660	CD2	PHE A 2		38.291	34.151	21.093		20.72	A
	MOTA	1661	CE1	PHE A 2	82	37.947	35.921	23.206	1.00	22.66	A
	ATOM	1662	CE2	PHE A 2	82	38.433	33.702	22.405	1.00	20.97	A
40	ATOM	1663	CZ	PHE A 2		38.261	34.590	23.466		19.58	А
	ATOM	1664	C	PHE A 2		36.169	36.263	17.503		24.39	A
	MOTA	1665	0	PHE A 2		36.802	35.585	16.694		25.80	A
	MOTA	1666	N	ARG A 2	83	35.355	37.248	17.142	1.00	24.99	A
	ATOM	1667	CA	ARG A 2	83	35.141	37.594	15.741	1.00	26.33	A
45	ATOM	1668	СВ	ARG A 2		33.721	37.209	15.316		28.91	А
73											
	MOTA	1669	CG	ARG A 2		33.293	35.808	15.724		30.27	A
	MOTA	1670	CD	ARG A 2	83	31.904	35.493	15.188	1.00	33.36	A
	ATOM	1671	NE	ARG A 2	83	30.890	36.392	15.733	1.00	32.76	A
	ATOM	1672	CZ	ARG A 2		30.372	36.287	16.952		34.79	А
50											
50	ATOM	1673		ARG A 2		30.767	35.317	17.768		35.77	A
	MOTA	1674	NH2	ARG A 2	83	29.458	37.156	17.359	1.00	36.12	A
	ATOM	1675	С	ARG A 2	83	35.328	39.096	15.544	1.00	26.47	A
	ATOM	1676	0	ARG A 2		35.029	39.888	16.438		26.28	А
	ATOM	1677	N	ALA A 2		35.818	39.486	14.373		26.70	A
55	MOTA	1678	CA	ALA A 2	84	36.033	40.899	14.079	1.00	27.84	A
	ATOM	1679	СВ	ALA A 2	84	37.188	41.442	14.914	1.00	26.24	A
	ATOM	1680	С	ALA A 2		36.327	41.077	12.602		28.35	А
	ATOM	1681	0	ALA A 2		36.560	40.101	11.891		29.91	A
	ATOM	1682	N	GLY A 2	85	36.332	42.329	12.153	T.00	29.29	A

	MOTA	1683	$^{\rm CA}$	GLY A	285	36.577	42.631	10.753	1.00 29.52	A
	MOTA	1684	С	GLY A	285	37.893	42.156	10.168	1.00 30.12	A
	ATOM	1685	0	GLY A	285	37.974	41.862	8.976	1.00 30.60	A
	ATOM	1686	N	ASN A		38.939	42.097	10.983	1.00 28.49	A
_										
5	ATOM	1687	CA	ASN A		40.231	41.644	10.489	1.00 26.71	A
	MOTA	1688	СВ	ASN A	286	41.050	42.825	9.945	1.00 26.11	A
	MOTA	1689	CG	ASN A	286	41.310	43.900	10.990	1.00 27.83	A
	ATOM	1690	OD1	ASN A	286	41.877	43.631	12.049	1.00 27.84	A
	ATOM	1691		ASN A		40.908	45.131	10.685	1.00 25.95	А
10	ATOM	1692	C	ASN A		40.997	40.924	11.584	1.00 26.03	A
10										
	MOTA	1693	0	ASN A		40.540	40.851	12.723	1.00 25.66	A
	ATOM	1694	N	GLU A		42.162	40.391	11.239	1.00 24.81	A
	MOTA	1695	CA	GLU A	287	42.965	39.662	12.206	1.00 27.59	A
	MOTA	1696	СВ	GLU A	287	44.145	38.985	11.510	1.00 30.17	A
15	ATOM	1697	CG	GLU A	287	43.776	37.632	10.931	1.00 38.21	А
	ATOM	1698	CD	GLU A		44.900	36.998	10.140	1.00 41.86	A
		1699		GLU A		46.061	37.036	10.608	1.00 43.08	
	ATOM									A
	ATOM	1700		GLU A		44.612	36.449	9.052	1.00 45.22	A
	ATOM	1701	С	GLU A		43.459	40.485	13.383	1.00 25.05	A
20	MOTA	1702	0	GLU A	287	43.382	40.030	14.521	1.00 26.41	A
	MOTA	1703	N	TYR A	288	43.966	41.685	13.122	1.00 23.04	A
	ATOM	1704	CA	TYR A	288	44.460	42.528	14.205	1.00 22.34	А
	ATOM	1705	СВ	TYR A		44.867	43.913	13.691	1.00 21.07	А
	ATOM	1706	CG	TYR A		45.275	44.858	14.805	1.00 21.07	A
25								15.405		
25	ATOM	1707		TYR A		46.533	44.762		1.00 21.23	A
	ATOM	1708		TYR A		46.891	45.588	16.475	1.00 20.43	A
	ATOM	1709	CD2	TYR A	288	44.380	45.809	15.302	1.00 22.32	A
	MOTA	1710	CE2	TYR A	288	44.725	46.637	16.373	1.00 23.28	A
	ATOM	1711	CZ	TYR A	288	45.981	46.518	16.953	1.00 22.96	A
30	ATOM	1712	OH	TYR A	288	46.316	47.313	18.024	1.00 23.18	A
	ATOM	1713	С	TYR A		43.402	42.698	15.288	1.00 21.38	A
	ATOM	1714	0	TYR A		43.710	42.616	16.473	1.00 22.09	A
				LEU A					1.00 21.88	
	ATOM	1715	N			42.159	42.939	14.874		A
	MOTA	1716	CA	LEU A		41.055	43.130	15.811	1.00 21.98	A
35	ATOM	1717	СВ	LEU A		39.821	43.673	15.078	1.00 22.90	A
	ATOM	1718	CG	LEU A	289	39.896	45.130	14.601	1.00 26.52	A
	MOTA	1719	CD1	LEU A	289	38.706	45.436	13.696	1.00 26.55	A
	MOTA	1720	CD2	LEU A	289	39.914	46.071	15.807	1.00 23.13	A
	ATOM	1721	С	LEU A	289	40.686	41.849	16.560	1.00 21.24	A
40	ATOM	1722	0	LEU A		40.256	41.897	17.715	1.00 20.72	А
.0	ATOM	1723	N	ILE A		40.843	40.708	15.900	1.00 19.62	A
										_
	ATOM	1724	CA	ILE A		40.538	39.433	16.533	1.00 18.54	A -
	MOTA	1725	СВ	ILE A		40.560	38.281	15.509	1.00 18.52	A
	MOTA	1726		ILE A		40.503	36.934	16.234	1.00 17.63	A
45	MOTA	1727	CG1	ILE A	290	39.378	38.429	14.545	1.00 18.88	A
	MOTA	1728	CD1	ILE A	290	39.421	37.483	13.357	1.00 19.81	A
	ATOM	1729	С	ILE A	290	41.578	39.167	17.618	1.00 19.09	A
	ATOM	1730	0	ILE A		41.236	38.788	18.737	1.00 18.20	A
	ATOM	1731	N	PHE A		42.849	39.376	17.286	1.00 18.76	A
50										
50	ATOM	1732	CA	PHE A		43.925	39.156	18.247	1.00 20.75	A
	ATOM	1733	СВ	PHE A		45.286	39.434	17.606	1.00 20.71	A
	MOTA	1734	CG	PHE A	291	45.644	38.480	16.503	1.00 22.92	A
	ATOM	1735	CD1	PHE A	291	45.065	37.214	16.443	1.00 22.98	A
	ATOM	1736	CD2	PHE A	291	46.588	38.830	15.543	1.00 22.91	A
55	ATOM	1737		PHE A		45.423	36.310	15.440	1.00 24.51	A
	ATOM	1738		PHE A		46.954	37.931	14.535	1.00 25.54	A
		1739	CZ							
	ATOM			PHE A		46.370	36.670	14.485	1.00 23.29	A
	ATOM	1740	С	PHE A		43.739	40.061	19.451	1.00 21.72	A
	ATOM	1741	0	PHE A	291	43.992	39.671	20.593	1.00 22.32	А

	ATOM	1742	N	GLN	Α	292	43.284	41.275	19.178	1.00	23.27	А
	ATOM	1743	CA	GLN			43.055	42.264	20.216		24.01	A
	ATOM	1744	СВ	GLN			42.574	43.559	19.562	1.00		А
	ATOM	1745	CG	GLN			42.577	44.773	20.447	1.00		A
5	ATOM	1746	CD	GLN			42.469	46.057	19.638	1.00		A
	ATOM	1747		GLN			41.520	46.244	18.872	1.00		A
	ATOM	1748		GLN			43.449	46.944	19.799		27.61	A
	ATOM	1749	C	GLN			42.018	41.733	21.204	1.00		A
	ATOM	1750	0	GLN			42.200	41.832	22.415	1.00		A
10	ATOM	1751	N	LYS			40.937	41.154	20.687	1.00		A
10	ATOM	1752	CA	LYS			39.895	40.612	21.558	1.00		A
	ATOM	1753	CB	LYS			38.664	40.223	20.740	1.00		A
	ATOM	1754	CG	LYS			37.919	41.407	20.740	1.00		A
	ATOM	1755	CD	LYS			36.651	40.961	19.429	1.00		A
15		1756		LYS			35.857	40.961	18.926	1.00		
13	ATOM	1757	CE	LYS			34.612	42.161	18.214	1.00		A
	ATOM		ΝZ				40.398					A
	ATOM	1758	C	LYS				39.398	22.343	1.00		A
	ATOM	1759	0			293	40.041	39.204	23.509		22.01	A
20	ATOM	1760	N	ILE			41.226	38.583	21.702	1.00		A
20	ATOM	1761	CA	ILE			41.774	37.394	22.347	1.00		A
	ATOM	1762	CB	ILE			42.631	36.575	21.349	1.00		A
	ATOM	1763		ILE			43.481	35.550	22.098	1.00		A
	ATOM	1764		ILE			41.716	35.897	20.318	1.00		A
25	ATOM	1765		ILE			42.467	35.237	19.178	1.00		A
23	ATOM	1766	C			294	42.618	37.727	23.587	1.00		A
	ATOM ATOM	1767	0	ILE			42.366	37.199	24.673	1.00		A
		1768 1769	N			295	43.610	38.600	23.439	1.00		A
	ATOM		CA			295	44.461	38.934	24.582	1.00		A
30	ATOM	1770 1771	CB	ILE		295	45.668 46.514	39.805 39.066	24.175 23.140	1.00		A A
30	ATOM ATOM	1772		ILE			45.189	41.151	23.140	1.00		A
	ATOM	1773		ILE			46.317	42.149	23.433	1.00		A
	ATOM	1774	CDI			295	43.720	39.636	25.717	1.00		A
	ATOM	1775	0	ILE			44.214	39.687	26.842	1.00		A
35	ATOM	1776	N	LYS			42.539	40.173	25.425	1.00		A
33	ATOM	1777	CA	LYS			41.743	40.173	26.444	1.00		A
		1778		LYS				40.033	25.894	1.00		
	ATOM	1779	CB	LYS			41.178	43.141		1.00		A
	MOTA	1780	CG						25.413		35.56	A
40	ATOM ATOM	1781	CD CE	LYS LYS			41.634 41.009	44.410 45.283	24.826 25.900	1.00		A A
40	ATOM	1782	NZ	LYS			40.564	46.603	25.357	1.00		A
		1783	C	LYS			40.593	39.958	26.893	1.00		
	ATOM ATOM	1784	_	LYS			39.770	40.361	27.713	1.00		A
	ATOM	1785	O	LEU			40.550	38.742	26.349	1.00		A A
45	ATOM	1786	CA	LEU			39.500	37.777	26.666	1.00		
43			CB	LEU						1.00		A
	ATOM	1787 1788					39.632	37.285	28.111			A
	ATOM ATOM	1789	CG CD1	LEU LEU			38.766	36.068 34.852	28.460 27.646	1.00		A
	ATOM	1790		LEU			39.238 38.856	35.777	29.951	1.00		A A
50	ATOM	1791	CDZ	LEU			38.151	38.459	26.467	1.00		A
50	ATOM	1792	0	LEU			37.261	38.378	27.309	1.00		A
	ATOM	1793	N	GLU			38.007	39.127	25.331	1.00		A
	ATOM	1794	CA	GLU			36.786	39.847	25.023	1.00		A
				GLU						1.00		
55	ATOM ATOM	1795 1796	CB CG	GLU			37.143 35.991	41.139 42.092	24.291 24.108	1.00		A z
55	ATOM	1796	CD	GLU			36.419	43.362	23.410	1.00		A A
	ATOM	1798		GLU			37.348	44.027	23.410	1.00		A
	ATOM	1799		GLU			35.832	43.693	22.359	1.00		A
	ATOM	1800	C	GLU			35.766	39.057	24.207	1.00		A
	ATON	T000	$\overline{}$	ОПО	17	200	55.700	55.057	44.407	1.00	20.19	A

	ATOM	1801	0	GLU	Α	298	35.832	39.017	22.979	1.00	24.35	Α
	ATOM	1802	N	TYR	Δ.	299	34.825	38.427	24.902	1.00	23 45	A
	ATOM	1803	CA	TYR			33.760	37.663	24.265	1.00		Α
	ATOM	1804	CB	TYR	Α	299	34.264	36.304	23.755	1.00	20.13	Α
5	ATOM	1805	CG	TYR	Δ	299	34.348	35.233	24.828	1.00	21 17	A
,							35.336			1.00		
	ATOM	1806		TYR				35.279	25.810			A
	ATOM	1807	CE1	TYR	Α	299	35.389	34.332	26.826	1.00	19.30	Α
	ATOM	1808	CD2	TYR	A	299	33.410	34.201	24.888	1.00	18.96	Α
	ATOM	1809		TYR			33.456	33.243	25.907	1.00		A
1.0												
10	ATOM	1810	CZ	TYR	А	299	34.449	33.321	26.870	1.00	18.79	А
	ATOM	1811	OH	TYR	Α	299	34.511	32.401	27.881	1.00	18.77	Α
	ATOM	1812	С	TYR	Α	299	32.699	37.437	25.331	1.00	25.20	Α
		1813						37.681				
	ATOM		0	TYR			32.942		26.506	1.00		Α
	ATOM	1814	N	ASP	Α	300	31.522	36.981	24.927	1.00	26.94	Α
15	ATOM	1815	CA	ASP	Α	300	30.467	36.710	25.891	1.00	30.60	Α
	ATOM	1816	СВ	ASP	Δ	300	29.665	37.981	26.179	1.00	35 86	Α
	ATOM	1817	CG	ASP			29.228	38.687	24.923	1.00		A
	ATOM	1818	OD1	ASP	Α	300	28.450	38.088	24.149	1.00	45.98	Α
	ATOM	1819	OD2	ASP	Α	300	29.666	39.840	24.707	1.00	45.69	Α
20	ATOM	1820	С	ASP			29.564	35.608	25.363	1.00	29 26	Α
20												
	ATOM	1821	0	ASP			29.590	35.299	24.172	1.00		A
	ATOM	1822	N	PHE	Α	301	28.778	35.011	26.253	1.00	28.96	Α
	ATOM	1823	CA	PHE	Α	301	27.884	33.924	25.871	1.00	30.48	Α
	ATOM	1824	СВ	PHE			27.818	32.854	26.968	1.00		A
2.5												
25	ATOM	1825	CG	PHE			29.147	32.279	27.356	1.00		Α
	ATOM	1826	CD1	PHE	Α	301	29.978	32.949	28.245	1.00	27.31	Α
	ATOM	1827	CD2	PHE	Α	301	29.560	31.050	26.845	1.00	27.89	Α
		1828		PHE						1.00		
	ATOM						31.205	32.403	28.625			Α
	ATOM	1829	CE2	PHE	Α	301	30.781	30.498	27.217	1.00	28.05	Α
30	ATOM	1830	CZ	PHE	Α	301	31.605	31.175	28.110	1.00	28.27	Α
	ATOM	1831	С	PHE	Δ	301	26.459	34.384	25.619	1.00	32 20	A
	ATOM	1832	0	PHE			25.946	35.261	26.317	1.00		А
	ATOM	1833	N	PRO	Α	302	25.798	33.804	24.607	1.00	33.29	Α
	ATOM	1834	CD	PRO	Α	302	26.313	32.943	23.529	1.00	34.04	A
35	ATOM	1835	CA	PRO			24.415	34.199	24.341	1.00		Α
33												
	ATOM	1836	СВ	PRO			24.144	33.608	22.959	1.00		A
	ATOM	1837	CG	PRO	Α	302	25.041	32.413	22.921	1.00	35.48	Α
	ATOM	1838	С	PRO	Α	302	23.567	33.561	25.444	1.00	37.39	A
	ATOM	1839	0	PRO			23.935	32.518	25.986	1.00		A
40												
40	ATOM	1840	N	ALA			22.447	34.188	25.783	1.00		А
	ATOM	1841	CA	ALA	Α	303	21.572	33.692	26.843	1.00	40.65	Α
	MOTA	1842	СВ	ALA	Α	303	20.280	34.506	26.862	1.00	41.66	A
	ATOM	1843	С	ALA			21.238	32.197	26.814	1.00		A
	ATOM	1844	0	ALA			21.253	31.537	27.854	1.00		А
45	ATOM	1845	N	ALA	Α	304	20.945	31.665	25.631	1.00	41.04	Α
	ATOM	1846	CA	ALA	Α	304	20.569	30.258	25.480	1.00	40.66	A
										1.00		
	ATOM	1847	СВ	ALA			20.121	30.004	24.040			A
	ATOM	1848	С	ALA	Α	304	21.628	29.223	25.876	1.00		Α
	ATOM	1849	0	ALA	Α	304	21.298	28.156	26.395	1.00	40.61	Α
50	ATOM	1850	N	PHE			22.891	29.543	25.617	1.00		А
•												
	ATOM	1851	CA	PHE			24.022	28.662	25.909	1.00		A
	MOTA	1852	СВ	PHE	Α	305	25.259	29.519	26.187	1.00	29.46	Α
	MOTA	1853	CG	PHE	Α	305	26.536	28.917	25.690	1.00	28.15	Α
	ATOM	1854		PHE			27.146	27.875	26.377	1.00		Α
55												
55	ATOM	1855		PHE			27.127	29.386	24.521	1.00		Α
	MOTA	1856	CE1	PHE	Α	305	28.330	27.308	25.908	1.00	26.92	Α
	MOTA	1857	CE2	PHE	Α	305	28.312	28.826	24.042	1.00	26.62	Α
	ATOM	1858	CZ	PHE			28.914	27.786	24.737	1.00		A
	ATOM	1859	С	PHE	А	303	23.811	27.664	27.057	1.00	30.09	Α

	ATOM	1860	0	PHE	Α	305	23.518	28.051	28.187	1.00 31.51	A
	ATOM	1861	N	PHE			23.964	26.378	26.758	1.00 27.01	A
	MOTA	1862	CA	PHE			23.801	25.334	27.769	1.00 26.30	A
	ATOM	1863	СВ	PHE	Α	306	24.157	23.970	27.170	1.00 25.03	A
5	ATOM	1864	CG	PHE	Α	306	23.548	23.725	25.815	1.00 27.24	A
	ATOM	1865	CD1	PHE	Α	306	22.170	23.831	25.622	1.00 28.40	A
	ATOM	1866	CD2	PHE	Α	306	24.350	23.386	24.728	1.00 27.84	A
	ATOM	1867	CE1	PHE	Α	306	21.601	23.603	24.365	1.00 28.05	A
	ATOM	1868	CE2	PHE	Α	306	23.792	23.155	23.465	1.00 28.31	A
10	ATOM	1869	CZ	PHE	Α	306	22.415	23.263	23.283	1.00 28.00	A
	ATOM	1870	С	PHE	A	306	24.711	25.652	28.961	1.00 26.23	А
	ATOM	1871	0	PHE	Α	306	25.927	25.775	28.811	1.00 25.59	A
	ATOM	1872	N	PRO	Α	307	24.125	25.796	30.163	1.00 26.67	A
	ATOM	1873	CD	PRO	Α	307	22.685	25.625	30.430	1.00 27.95	А
15	ATOM	1874	CA	PRO	Α	307	24.842	26.110	31.405	1.00 26.59	А
	ATOM	1875	СВ	PRO	Α	307	23.795	25.832	32.481	1.00 26.14	A
	ATOM	1876	CG	PRO	Α	307	22.531	26.250	31.803	1.00 27.86	A
	ATOM	1877	С	PRO	Α	307	26.145	25.355	31.659	1.00 25.58	A
	ATOM	1878	0	PRO	Α	307	27.189	25.964	31.900	1.00 22.65	A
20	ATOM	1879	N	LYS	Α	308	26.085	24.031	31.620	1.00 24.46	A
	ATOM	1880	CA	LYS	Α	308	27.274	23.232	31.867	1.00 23.91	A
	ATOM	1881	СВ	LYS	Α	308	26.887	21.760	32.024	1.00 23.25	A
	ATOM	1882	CG	LYS	Α	308	26.062	21.532	33.285	1.00 28.49	A
	ATOM	1883	CD	LYS	Α	308	25.618	20.093	33.466	1.00 30.17	A
25	ATOM	1884	CE	LYS	Α	308	24.760	19.973	34.722	1.00 33.12	A
	ATOM	1885	NZ	LYS	Α	308	24.122	18.636	34.860	1.00 34.13	A
	ATOM	1886	С	LYS	Α	308	28.314	23.426	30.769	1.00 22.84	A
	ATOM	1887	0	LYS	Α	308	29.514	23.411	31.042	1.00 22.46	A
	ATOM	1888	N	ALA	Α	309	27.861	23.621	29.534	1.00 21.59	A
30	ATOM	1889	CA	ALA	Α	309	28.792	23.848	28.432	1.00 20.02	A
	ATOM	1890	СВ	ALA	A	309	28.056	23.856	27.106	1.00 18.80	A
	ATOM	1891	С	ALA	Α	309	29.481	25.191	28.662	1.00 21.41	A
	ATOM	1892	0	ALA	Α	309	30.680	25.335	28.427	1.00 21.39	A
	ATOM	1893	N	ARG	Α	310	28.717	26.179	29.121	1.00 21.39	A
35	ATOM	1894	CA	ARG	Α	310	29.290	27.494	29.388	1.00 22.02	A
	ATOM	1895	СВ	ARG	Α	310	28.213	28.479	29.854	1.00 22.39	A
	ATOM	1896	CG	ARG	Α	310	28.806	29.756	30.436	1.00 25.30	A
	ATOM	1897	CD	ARG	Α	310	27.780	30.852	30.664	1.00 28.33	A
	ATOM	1898	NE	ARG	Α	310	28.420	32.039	31.230	1.00 30.18	A
40	ATOM	1899	CZ	ARG	Α	310	27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900	NH1	ARG	Α	310	26.719	33.477	30.634	1.00 31.19	A
	ATOM	1901	NH2	ARG	Α	310	28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	С	ARG	Α	310	30.376	27.388	30.458	1.00 21.65	A
	ATOM	1903	0	ARG	Α	310	31.464	27.949	30.311	1.00 20.36	A
45	ATOM	1904	N	ASP	Α	311	30.074	26.677	31.541	1.00 19.57	A
	ATOM	1905	CA	ASP	Α	311	31.043	26.512	32.615	1.00 20.18	A
	ATOM	1906	СВ	ASP	Α	311	30.460	25.649	33.739	1.00 20.39	A
	ATOM	1907	CG	ASP			31.439	25.446	34.881	1.00 23.35	А
	ATOM	1908	OD1	ASP			32.158	24.428	34.885	1.00 24.91	А
50	ATOM	1909		ASP			31.500	26.312	35.776	1.00 26.96	А
	ATOM	1910	С	ASP			32.322	25.877	32.073	1.00 19.73	А
	ATOM	1911	0	ASP			33.422	26.289	32.439	1.00 19.30	А
	ATOM	1912	N	LEU			32.179	24.891	31.188	1.00 16.32	A
	ATOM	1913	CA	LEU			33.349	24.226	30.611	1.00 16.66	А
55	ATOM	1914	СВ	LEU			32.927	23.035	29.744	1.00 16.12	A
	ATOM	1915	CG	LEU			34.050	22.320	28.974	1.00 14.73	А
	ATOM	1916		LEU			35.192	21.935	29.912	1.00 14.56	A
	ATOM	1917		LEU			33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	С	LEU			34.181	25.189	29.774	1.00 16.61	А

	ATOM	1919	0	LEU	Α	312	35.402	25.241	29.910	1.00	16.20	A
	ATOM	1920	N	VAL			33.515	25.949	28.908		16.20	А
	ATOM	1921	CA	VAL	Α	313	34.207	26.907	28.058	1.00	15.37	A
	ATOM	1922	CB	VAL	Α	313	33.216	27.648	27.130	1.00	16.42	A
5	ATOM	1923	CG1	VAL			33.915	28.796	26.426		16.93	А
5												
	ATOM	1924	CG2	VAL			32.644	26.672	26.103		17.88	A
	ATOM	1925	С	VAL	Α	313	34.960	27.923	28.911	1.00	17.39	A
	ATOM	1926	0	VAL	Ά	313	36.093	28.294	28.591	1.00	18.00	А
											17.61	
	ATOM	1927	N	GLU			34.342	28.364	30.004			А
10	MOTA	1928	CA	GLU	Α	314	34.986	29.331	30.885	1.00	20.43	A
	ATOM	1929	СВ	GLU	Α	314	34.009	29.816	31.959	1.00	22.14	A
	ATOM	1930	CG	GLU			32.800	30.550	31.396		26.52	А
	ATOM	1931	CD	GLU			31.852	31.025	32.478		31.26	A
	ATOM	1932	OE 1	GLU	Α	314	31.580	30.246	33.417	1.00	33.48	A
15	ATOM	1933	OE2	GLU	Α	314	31.370	32.173	32.387	1.00	34.81	А
15		1934		GLU			36.217	28.721				
	ATOM		С						31.539		19.15	A
	ATOM	1935	0	GLU	Α	314	37.134	29.433	31.934	1.00	21.47	A
	ATOM	1936	N	LYS	Α	315	36.245	27.400	31.651	1.00	19.51	A
	ATOM	1937	CA	LYS	Ζ.	315	37.394	26.749	32.258	1 00	19.17	А
20												
20	ATOM	1938	СВ	LYS			36.946	25.514	33.043		18.84	A
	ATOM	1939	CG	LYS	Α	315	36.280	25.885	34.368	1.00	19.62	A
	ATOM	1940	CD	LYS	Α	315	35.653	24.696	35.073	1.00	19.22	А
		1941	CE	LYS			35.070	25.095	36.427		21.00	A
	ATOM											
	ATOM	1942	NZ	LYS			36.119	25.552	37.381	1.00	19.53	A
25	ATOM	1943	С	LYS	Α	315	38.452	26.393	31.218	1.00	18.96	A
	ATOM	1944	0	LYS	Δ	315	39.511	25.873	31.561	1 00	19.85	А
											17.08	
	ATOM	1945	N	LEU			38.164	26.691	29.950			A
	ATOM	1946	CA	LEU	Α	316	39.102	26.429	28.854	1.00	16.41	A
	ATOM	1947	СВ	LEU	Α	316	38.414	25.636	27.738	1.00	13.81	A
30	ATOM	1948	CG	LEU			38.028	24.201	28.115		14.39	A
30												
	ATOM	1949		LEU			37.139	23.597	27.031		12.38	A
	ATOM	1950	CD2	LEU	Α	316	39.302	23.373	28.309	1.00	12.77	A
	ATOM	1951	С	LEU	Α	316	39.652	27.743	28.290	1.00	17.12	A
	ATOM	1952		LEU			40.851	27.860	28.023		16.53	A
			0									
35	ATOM	1953	N	LEU	Α	317	38.780	28.729	28.105	1.00	16.27	A
	ATOM	1954	CA	LEU	Α	317	39.228	30.022	27.596	1.00	17.52	A
	ATOM	1955	СВ	LEU	Δ	317	38.083	30.752	26.887	1 00	16.37	А
	ATOM	1956	CG	LEU			37.448	29.973	25.727		18.81	A
	ATOM	1957	CD1	LEU	Α	317	36.415	30.851	25.018	1.00	16.47	A
40	ATOM	1958	CD2	LEU	Α	317	38.528	29.526	24.741	1.00	17.87	A
	ATOM	1959	С	LEU			39.745	30.841	28.774		18.27	А
	ATOM	1960	0	LEU			39.078	31.753	29.273		18.58	A
	MOTA	1961	N	VAL	Α	318	40.937	30.475	29.229	1.00	18.02	A
	MOTA	1962	CA	VAL	Α	318	41.593	31.141	30.342	1.00	18.85	A
45	ATOM	1963	СВ	VAL			41.846	30.153	31.500		19.91	A
73												
	ATOM	1964	CGI	VAL	Α	318	42.590	30.848	32.634	1.00	20.01	A
	ATOM	1965	CG2	VAL	Α	318	40.520	29.584	31.990	1.00	19.44	A
	ATOM	1966	С	VAL	Ά	318	42.923	31.657	29.811	1.00	19.67	A
	ATOM	1967	0	VAL			43.690	30.902	29.208		18.26	А
50	MOTA	1968	N	LEU	Α	319	43.197	32.939	30.028	1.00	20.07	A
	MOTA	1969	CA	LEU	Α	319	44.436	33.533	29.538	1.00	20.98	A
	ATOM	1970	СВ	LEU			44.521	35.002	29.968		21.64	А
	ATOM	1971	CG	LEU			43.418	35.908	29.408		24.38	A
	ATOM	1972	CD1	LEU	Α	319	43.606	37.332	29.935	1.00	23.28	A
55	ATOM	1973		LEU			43.453	35.887	27.875	1.00	24.33	А
		1974		LEU								
	ATOM		C				45.680	32.774	29.994		20.38	A
	ATOM	1975	0	LEU	А	319	46.568	32.496	29.192		21.34	A
	ATOM	1976	N	ASP	Α	320	45.742	32.440	31.280	1.00	20.22	A
	ATOM	1977	CA	ASP			46.879	31.707	31.833		20.90	А
	211 01.1	エ フ 1 1	∪ 17	110 L	11	520	10.010	J. 101	51.055	1. 00	20.00	А

	ATOM	1978	СВ	ASP	А	320	46.842	31.760	33.365	1.00	20.76	А
	ATOM	1979	CG	ASP			48.049	31.102	34.004		21.51	A
	ATOM	1980		ASP			48.669	30.226	33.367		23.46	A
	ATOM	1981		ASP			48.371	31.450	35.159		23.89	A
5	ATOM	1982	C	ASP			46.814	30.247	31.367		20.06	A
5	ATOM	1983	0	ASP			45.988	29.476	31.840		20.54	A
		1983		ALA			47.700				20.68	
	ATOM		N					29.876	30.451			A
	ATOM	1985	CA	ALA			47.733	28.522	29.903		22.04	A
10	ATOM	1986	СВ	ALA			48.860	28.411	28.881		20.75	A
10	ATOM	1987	С	ALA			47.858	27.400	30.940		21.62	A
	MOTA	1988	0	ALA			47.482	26.259	30.665		21.99	A
	ATOM	1989	N	THR			48.372	27.715	32.127		20.89	A
	ATOM	1990	CA	THR			48.531	26.698	33.167		20.82	A
	MOTA	1991	СВ	THR			49.670	27.051	34.146		19.47	A
15	ATOM	1992	OG1	THR	Α	322	49.341	28.253	34.848	1.00	20.19	A
	MOTA	1993	CG2	THR	А	322	50.981	27.249	33.394	1.00	21.59	A
	ATOM	1994	С	THR	Α	322	47.264	26.498	33.983	1.00	19.55	A
	MOTA	1995	0	THR	Α	322	47.235	25.673	34.894	1.00	21.13	A
	MOTA	1996	N	LYS	Α	323	46.216	27.248	33.661	1.00	19.33	A
20	ATOM	1997	CA	LYS	Α	323	44.962	27.122	34.392	1.00	21.20	A
	ATOM	1998	СВ	LYS	Α	323	44.580	28.460	35.030	1.00	23.75	A
	ATOM	1999	CG	LYS			45.562	28.933	36.084	1.00	28.45	А
	ATOM	2000	CD	LYS			45.055	30.177	36.799		33.76	А
	ATOM	2001	CE	LYS			46.087	30.678	37.802		36.15	A
25	ATOM	2002	NZ	LYS			46.532	29.569	38.693		37.34	A
	ATOM	2003	C	LYS			43.806	26.614	33.539		20.68	A
	ATOM	2004	0	LYS			42.649	26.757	33.915		20.42	A
	ATOM	2005	N	ARG			44.114	26.019	32.392		19.97	A
	ATOM	2005	CA	ARG			43.060	25.494	31.531		17.98	A
30	ATOM	2007	CB	ARG			43.461	25.609	30.061		15.95	A
30		2007					43.534				17.34	
	ATOM		CG	ARG				27.050	29.603			A
	ATOM	2009	CD	ARG			43.996	27.194	28.172		19.80	A
	ATOM	2010	NE	ARG			44.438	28.565	27.944		16.93	A
2.5	ATOM	2011	CZ	ARG			45.410	28.908	27.108		19.88	A
35	ATOM	2012		ARG			46.045	27.978	26.398		14.58	A
	MOTA	2013		ARG			45.774	30.181	27.015		16.51	A
	ATOM	2014	С	ARG			42.762	24.046	31.883		18.32	A
	ATOM	2015	0	ARG			43.673	23.222	32.006		18.20	A
	ATOM	2016	N	LEU			41.479	23.748	32.055		18.32	A
40	ATOM	2017	CA	LEU			41.050	22.403	32.395		17.79	A
	MOTA	2018	CB	LEU	Α	325	39.523	22.335	32.425	1.00	17.03	A
	MOTA	2019	CG	LEU	Α	325	38.896	21.125	33.116	1.00	15.91	A
	ATOM	2020	CD1	LEU	Α	325	39.392	21.048	34.557	1.00	15.93	A
	ATOM	2021	CD2	LEU	Α	325	37.375	21.255	33.084	1.00	16.56	A
45	ATOM	2022	С	LEU	Α	325	41.599	21.433	31.356	1.00	18.68	A
	ATOM	2023	0	LEU	Α	325	41.347	21.586	30.157	1.00	18.28	A
	ATOM	2024	N	GLY	Α	326	42.354	20.439	31.821	1.00	18.18	A
	ATOM	2025	CA	GLY			42.931	19.462	30.915	1.00	16.36	A
	ATOM	2026	С	GLY			44.443	19.558	30.807		19.15	А
50	ATOM	2027	0			326	45.093	18.592	30.404		19.52	А
	ATOM	2028	N	CYS			45.016	20.708	31.161		18.16	А
	ATOM	2029	CA	CYS			46.463	20.867	31.075		19.30	A
	ATOM	2030	CB	CYS			46.856	22.350	31.058		20.22	A
	ATOM	2030	SG	CYS			46.782	23.200	32.649		21.97	A
55	ATOM	2031	C	CYS			47.169	20.157	32.228		20.22	
55		2032					46.561	19.828	33.246		17.92	A
	ATOM		O N	CYS								A
	ATOM	2034	N	GLU			48.463	19.933	32.053		20.51	A
	ATOM	2035	CA	GLU			49.274	19.244	33.042		23.34	A
	ATOM	2036	СВ	GLU	А	328	50.710	19.139	32.507	1.00	28.68	А

	ATOM	2037	CG	GLU			50.754	18.367	31.175	1.00 38.24	A
	ATOM	2038	CD	GLU			52.067	18.500	30.414	1.00 43.23	A -
	ATOM	2039		GLU			52.535	19.643	30.218	1.00 46.22	A
-	ATOM	2040	OE2				52.618	17.459	29.991	1.00 44.90	A
5	ATOM	2041	С	GLU			49.234	19.876	34.435	1.00 22.11	A
	ATOM	2042	0	GLU			49.147	19.161	35.437	1.00 20.27	A
	ATOM	2043	N	GLU			49.276	21.204	34.506	1.00 18.40	A
	ATOM	2044	CA	GLU			49.248	21.875	35.801	1.00 20.13	A
10	ATOM	2045	CB	GLU			49.587	23.363	35.657	1.00 20.36	A
10	ATOM	2046	CG	GLU			51.014	23.651	35.190	1.00 24.05 1.00 25.93	A
	ATOM	2047	CD	GLU			51.191	23.518	33.688		A
	ATOM	2048		GLU			50.213	23.154	32.995	1.00 26.61 1.00 27.19	A
	ATOM	2049 2050	OE2	GLU GLU			52.311	23.781	33.198		A
15	ATOM		C				47.890	21.718	36.480	1.00 19.36	A
15	ATOM ATOM	2051 2052	O	GLU MET			47.775 46.863	21.879 21.415	37.694 35.691	1.00 18.74 1.00 17.28	A A
		2052	N	MET			45.520	21.413	36.229	1.00 17.28	
	ATOM	2053	CA								A
	ATOM	2054	CB	MET MET			44.474 44.460	21.833 23.365	35.294 35.311	1.00 17.65 1.00 22.95	A
20	ATOM ATOM	2056	CG SD	MET			44.460	24.026	36.979	1.00 22.93	A A
20	ATOM	2057	CE	MET			42.435	23.712	37.186	1.00 24.69	A
	ATOM	2057	CE	MET			45.257	19.730	36.422	1.00 24.09	A
	ATOM	2059	0	MET			44.127	19.730	36.629	1.00 14.30	A
	ATOM	2060	N	GLU			46.327	18.949	36.346	1.00 15.39	A
25	ATOM	2061	CA	GLU			46.289	17.501	36.531	1.00 17.08	A
23	ATOM	2062	CB	GLU			45.607	17.155	37.862	1.00 17.00	A
	ATOM	2063	CG	GLU			46.070	18.027	39.038	1.00 17.46	A
	ATOM	2064	CD	GLU			47.591	18.179	39.145	1.00 20.16	A
	ATOM	2065		GLU			48.034	19.073	39.896	1.00 21.39	A
30	ATOM	2066		GLU			48.345	17.420	38.500	1.00 18.87	A
30	ATOM	2067	C	GLU			45.697	16.658	35.398	1.00 17.80	A
	ATOM	2068	0	GLU			45.107	15.602	35.636	1.00 20.40	A
	ATOM	2069	N	GLY			45.844	17.133	34.167	1.00 16.23	A
	ATOM	2070	CA	GLY			45.420	16.353	33.015	1.00 14.10	A
35	ATOM	2071	C	GLY			43.982	16.154	32.596	1.00 13.54	A
-	ATOM	2072	0	GLY			43.063	16.864	33.017	1.00 11.96	A
	ATOM	2073	N	TYR			43.804	15.141	31.750	1.00 14.37	A
	ATOM	2074	CA	TYR			42.510	14.806	31.182	1.00 13.56	A
	ATOM	2075	СВ	TYR			42.722	13.892	29.968	1.00 15.00	A
40	ATOM	2076	CG	TYR			43.153	14.683	28.752	1.00 16.46	А
	ATOM	2077	CD1	TYR	Α	333	42.206	15.172	27.849	1.00 15.29	A
	ATOM	2078	CE1	TYR	Α	333	42.573	16.002	26.794	1.00 13.42	A
	ATOM	2079	CD2	TYR	Α	333	44.490	15.039	28.561	1.00 14.91	A
	ATOM	2080		TYR			44.872	15.877	27.499	1.00 14.87	A
45	ATOM	2081	CZ	TYR	Α	333	43.902	16.353	26.626	1.00 15.61	A
	ATOM	2082	OH	TYR	Α	333	44.244	17.197	25.599	1.00 17.29	A
	ATOM	2083	С	TYR	Α	333	41.470	14.230	32.127	1.00 15.23	A
	MOTA	2084	0	TYR	Α	333	40.278	14.323	31.846	1.00 16.63	A
	MOTA	2085	N	GLY	Α	334	41.907	13.650	33.244	1.00 15.50	A
50	MOTA	2086	CA	GLY	Α	334	40.957	13.100	34.202	1.00 15.07	A
	MOTA	2087	С	GLY	Α	334	39.925	14.146	34.616	1.00 16.40	A
	MOTA	2088	0	GLY	А	334	38.724	13.946	34.433	1.00 15.05	A
	MOTA	2089	N	PRO	Α	335	40.366	15.278	35.184	1.00 14.96	A
	ATOM	2090	CD	PRO	Α	335	41.727	15.531	35.689	1.00 15.88	A
55	MOTA	2091	CA	PRO	Α	335	39.444	16.339	35.606	1.00 15.29	A
	MOTA	2092	СВ	PRO			40.383	17.397	36.178	1.00 13.19	A
	MOTA	2093	CG	PRO			41.485	16.569	36.758	1.00 13.81	A
	MOTA	2094	С	PRO			38.594	16.877	34.448	1.00 15.84	А
	MOTA	2095	0	PRO	Α	335	37.423	17.204	34.631	1.00 14.84	А

	ATOM	2096	N	LEU			39.184	16.971	33.257	1.00 16.12	А
	ATOM	2097	CA	LEU			38.450	17.465	32.094	1.00 15.52	A
	ATOM	2098	СВ	LEU			39.396	17.653	30.898	1.00 14.39	A
	ATOM	2099	CG	LEU			38.770	17.991	29.538	1.00 15.46	A
5	ATOM	2100		LEU			37.836	19.182	29.662	1.00 11.25	A
	ATOM	2101	CD2	LEU	Α	336	39.884	18.285	28.528	1.00 14.11	A
	ATOM	2102	С			336	37.321	16.508	31.714	1.00 16.28	A
	ATOM	2103	0	LEU	Α	336	36.176	16.921	31.540	1.00 15.51	A
	MOTA	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00 17.22	A
10	MOTA	2105	CA	LYS	Α	337	36.624	14.243	31.235	1.00 17.39	A
	ATOM	2106	СВ	LYS			37.293	12.900	30.921	1.00 17.68	A
	ATOM	2107	CG	LYS			38.170	12.994	29.676	1.00 22.31	A
	ATOM	2108	CD	LYS			39.213	11.892	29.592	1.00 24.60	A
	ATOM	2109	CE	LYS			38.620	10.560	29.189	1.00 24.76	A
15	ATOM	2110	NZ	LYS			39.710	9.560	28.997	1.00 25.05	А
	ATOM	2111	С	LYS			35.577	14.096	32.342	1.00 17.33	A
	ATOM	2112	0	LYS	А	337	34.456	13.652	32.090	1.00 14.42	А
	ATOM	2113	N	ALA			35.928	14.500	33.559	1.00 15.83	A
	ATOM	2114	CA	ALA			34.989	14.395	34.674	1.00 17.52	A
20	ATOM	2115	СВ	ALA			35.749	14.167	35.980	1.00 19.68	A
	ATOM	2116	С	ALA			34.095	15.621	34.804	1.00 18.83	A
	ATOM	2117	0	ALA			33.252	15.687	35.695	1.00 18.94	A
	ATOM	2118	N	HIS			34.262	16.596	33.918	1.00 19.42	A
	ATOM	2119	CA	HIS			33.438	17.796	34.004	1.00 19.28	A
25	ATOM	2120	СВ	HIS			33.865	18.819	32.949	1.00 19.20	A
	MOTA	2121	CG	HIS			33.163	20.134	33.074	1.00 20.26	A
	ATOM	2122	CD2	HIS	Α	339	33.549	21.299	33.649	1.00 18.95	A
	ATOM	2123		HIS			31.880	20.340	32.612	1.00 19.10	A
	ATOM	2124		HIS			31.506	21.576	32.896	1.00 22.19	A
30	ATOM	2125		HIS			32.500	22.179	33.525	1.00 21.98	A
	MOTA	2126	С	HIS			31.957	17.448	33.845	1.00 19.13	A
	ATOM	2127	0	HIS			31.597	16.576	33.061	1.00 19.52	A
	MOTA	2128	N			340	31.079	18.125	34.606	1.00 19.80	A
	ATOM	2129	CD	PRO			31.424	19.119	35.640	1.00 19.08	A
35	MOTA	2130	CA	PRO			29.630	17.900	34.569	1.00 20.52	A
	MOTA	2131	СВ			340	29.091	19.058	35.396	1.00 20.74	A
	MOTA	2132	CG	PRO			30.146	19.207	36.454	1.00 19.20	A
	MOTA	2133	С	PRO			29.000	17.834	33.176	1.00 21.42	A
	ATOM	2134	0	PRO			28.049	17.088	32.955	1.00 22.48	A
40	MOTA	2135	N			341	29.528	18.606	32.237	1.00 21.33	А
	MOTA	2136	CA			341	28.985	18.610	30.886	1.00 21.57	A
	MOTA	2137	СВ			341	29.739	19.624	30.017	1.00 21.64	A
	ATOM	2138	CG	PHE			29.207	19.740	28.613	1.00 23.18	A
	MOTA	2139		PHE			27.903	20.171	28.382	1.00 22.58	A
45	MOTA	2140		PHE			30.013	19.431	27.522	1.00 21.95	А
	ATOM	2141		PHE			27.410	20.292	27.082	1.00 23.54	A
	ATOM	2142		PHE			29.533	19.548	26.220	1.00 21.83	A
	MOTA	2143	CZ	PHE			28.228	19.980	25.998	1.00 23.23	A
	MOTA	2144	С	PHE			29.055	17.226	30.237	1.00 21.84	A
50	ATOM	2145	0			341	28.232	16.896	29.389	1.00 20.37	А
	MOTA	2146	N	PHE			30.034	16.422	30.640	1.00 20.51	A
	ATOM	2147	CA	PHE			30.221	15.085	30.077	1.00 23.01	А
	ATOM	2148	СВ	PHE			31.710	14.809	29.850	1.00 18.00	A
	ATOM	2149	CG	PHE			32.398	15.812	28.971	1.00 17.05	A
55	ATOM	2150		PHE			32.010	15.987	27.652	1.00 17.78	A
	ATOM	2151		PHE			33.487	16.534	29.450	1.00 15.72	A
	ATOM	2152		PHE			32.702	16.867	26.811	1.00 18.08	A
	ATOM	2153		PHE			34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ	PHE	A	342	33.790	17.578	27.298	1.00 16.56	А

	ATOM	2155	С	PHE	Α	342	29.679	13.972	30.976	1.00 24	. 95	Α
	7) III O N f	2156		PHE	7\	242				1 00 22	0.5	
	MOTA		0				30.002	12.798	30.777	1.00 23		A
	ATOM	2157	N	GLU	Α	343	28.861	14.333	31.958	1.00 27	.35	Α
	ATOM	2158	CA	GLU	Δ	343	28.325	13.349	32.897	1.00 30	28	Α
-												
5	ATOM	2159	СВ	GLU			27.187	13.964	33.716	1.00 32		Α
	ATOM	2160	CG	GLU	Α	343	26.581	12.991	34.714	1.00 39	.71	Α
	ATOM	2161	CD	GLU	7\	3/13	25.628	13.661	35.688	1.00 44	72	Α
	MOTA	2162	OET	GLU	А	343	24.661	14.314	35.234	1.00 47	.55	Α
	ATOM	2163	OE2	GLU	Α	343	25.847	13.526	36.911	1.00 46	.89	Α
10	ATOM	2164	С	GLU			27.852	12.017	32.305	1.00 28		А
10												
	ATOM	2165	0	GLU	Α	343	28.225	10.952	32.800	1.00 31		Α
	ATOM	2166	N	SER	Α	344	27.037	12.067	31.258	1.00 26	.09	Α
		2167		SER			26.520	10.838	30.656	1.00 28		
	MOTA		CA									Α
	ATOM	2168	СВ	SER	Α	344	25.129	11.089	30.067	1.00 28	.73	Α
15	ATOM	2169	OG	SER	Α	344	25.203	11.942	28.940	1.00 30	. 91	Α
	ATOM	2170	С	SER			27.407	10.214	29.577	1.00 27		A
	ATOM	2171	0	SER	Α	344	26.987	9.281	28.900	1.00 28	.66	Α
	ATOM	2172	N	VAL	Δ	345	28.627	10.715	29.419	1.00 26	75	Α
										1.00 23		
	MOTA	2173	CA	VAL			29.534	10.183	28.402			Α
20	ATOM	2174	CB	VAL	Α	345	30.565	11.256	27.950	1.00 23	.10	Α
	ATOM	2175	CG1	VAL	Δ	345	31.589	10.631	26.995	1.00 22	24	Α
	ATOM	2176	CGZ	VAL			29.854	12.418	27.275	1.00 20		Α
	ATOM	2177	С	VAL	Α	345	30.326	8.957	28.855	1.00 24	.26	Α
	ATOM	2178	0	VAL			30.876	8.930	29.960	1.00 22	83	Α
2.5												
25	ATOM	2179	N	THR	А	346	30.374	7.942	27.997	1.00 21	. / /	Α
	ATOM	2180	CA	THR	Α	346	31.153	6.740	28.272	1.00 23	.70	Α
	ATOM	2181	СВ	THR	7	346	30.391	5.455	27.857	1.00 26	53	Α
	ATOM	2182	OGI	THR	А	346	29.248	5.284	28.706	1.00 29	.98	Α
	ATOM	2183	CG2	THR	Α	346	31.289	4.231	27.990	1.00 24	.28	Α
30	ATOM	2184	С	THR			32.383	6.945	27.385	1.00 23		Α
30												
	ATOM	2185	0	THR	Α	346	32.306	6.827	26.160	1.00 24	.50	Α
	ATOM	2186	N	TRP	Α	347	33.508	7.270	28.013	1.00 22	.98	Α
	ATOM	2187	CA	TRP			34.744	7.569	27.300	1.00 23		A
	ATOM	2188	CB	TRP	Α	347	35.683	8.352	28.219	1.00 22	.54	Α
35	ATOM	2189	CG	TRP	Α	347	35.128	9.658	28.693	1.00 20	.61	Α
	ATOM	2190		TRP			35.257	10.927	28.040	1.00 19		A
	ATOM	2191	CE2	TRP	Α	347	34.581	11.881	28.838	1.00 18	.39	Α
	ATOM	2192	CE3	TRP	Α	347	35.878	11.351	26.858	1.00 18	.16	Α
		2193		TRP			34.397	9.883	29.828	1.00 18		A
	ATOM											
40	ATOM	2194	NE1	TRP	Α	347	34.065	11.218	29.923	1.00 19	.51	Α
	ATOM	2195	CZ2	TRP	Α	347	34.510	13.234	28.491	1.00 16	.88	Α
	ATOM	2196	CZ3				35.808	12.701	26.511	1.00 17		
												A
	ATOM	2197	CH2	TRP	Α	347	35.127	13.624	27.327	1.00 18		Α
	ATOM	2198	С	TRP	Α	347	35.538	6.429	26.675	1.00 25	.79	Α
45	ATOM	2199	0	TRP			36.304	6.654	25.742	1.00 24		А
45												
	ATOM	2200	N	ALA	Α	348	35.360	5.215	27.183	1.00 27	.10	Α
	ATOM	2201	CA	ALA	Α	348	36.116	4.063	26.697	1.00 27	.46	Α
				ALA								
	MOTA	2202	СВ				35.899	2.869	27.636	1.00 27		A
	ATOM	2203	С	ALA	Α	348	35.895	3.620	25.256	1.00 27	.18	Α
50	ATOM	2204	0	ALA	А	348	36.830	3.148	24.613	1.00 29	.41	Α
•				ASN								
	MOTA	2205	N				34.682	3.769	24.735	1.00 26		A
	ATOM	2206	CA	ASN	Α	349	34.418	3.310	23.375	1.00 27	.28	Α
	ATOM	2207	СВ	ASN			33.700	1.962	23.444	1.00 29	. 37	Α
	MOTA	2208	CG	ASN			32.299	2.088	24.013	1.00 30		А
55	ATOM	2209	OD1	ASN	Α	349	32.045	2.942	24.859	1.00 30	.17	Α
	ATOM	2210	ND2	ASN	Α	349	31.386	1.237	23.553	1.00 33		Α
	MOTA	2211	С	ASN			33.599	4.265	22.509	1.00 26		Α
	ATOM	2212	0	ASN	Α	349	32.669	3.843	21.819	1.00 25	.87	Α
	ATOM	2213	N	LEU	Ά	350	33.947	5.543	22.518	1.00 24		Α
	111 011	2210	**	0	- 1		55.517	0.010		1.00 21	. 10	4.1

	ATOM	2214	CA	LEU	Α	350	33.203	6.510	21.721	1.00 23.14	A
	ATOM	2215	СВ			350	33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU			33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217		LEU			34.646	9.756	23.293	1.00 19.36	A
5	ATOM	2218		LEU			32.220	9.094	23.319	1.00 18.78	A
	ATOM	2219	C			350	33.082	6.152	20.240	1.00 22.60	A
	ATOM	2220	0	LEU			32.011	6.296	19.650	1.00 21.15	A
	ATOM	2221	N	HIS			34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS			34.089	5.387	18.204	1.00 27.83	A
10	ATOM	2223	CB	HIS			35.506	5.325	17.596	1.00 29.36	A
10	ATOM	2224	CG	HIS			36.082	3.950	17.493	1.00 32.07	A
	ATOM	2225		HIS			36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226		HIS			36.197	3.285	16.291	1.00 32.03	A
	ATOM	2227		HIS			36.775	2.113	16.493	1.00 33.58	A
15	ATOM	2228		HIS			37.036	1.992	17.782	1.00 33.36	A
15	ATOM	2229	С	HIS			33.258	4.144	17.702	1.00 31.70	A
	ATOM	2230	0	HIS			33.015	3.847	16.707	1.00 20.12	A
	ATOM	2231	N	GLN			32.800	3.442	18.908	1.00 29.28	A
	ATOM	2232	CA	GLN			31.963	2.255	18.726	1.00 29.67	A
20	ATOM	2233	CB	GLN			32.366	1.145	19.694	1.00 29.07	A
20	ATOM	2234	CG	GLN			33.169	0.041	19.034	1.00 30.88	A
	ATOM	2234	CD	GLN			34.493	-0.186	19.729	1.00 30.00	A
	ATOM	2236		GLN			34.541	-0.450	20.928	1.00 31.21	A
		2237		GLN			35.578	-0.430	18.971	1.00 30.70	
25	ATOM ATOM	2237	C	GLN			30.504	2.638	18.963	1.00 32.30	A A
23		2239		GLN			29.595	1.831	18.770	1.00 30.42	
	ATOM	2239	O	GLN			30.290	3.875	19.397	1.00 29.01	A
	ATOM	2240	N					4.365		1.00 27.64	A
	ATOM	2241	CA			353	28.948		19.652	1.00 27.42	A
20	ATOM		CB			353	28.977	5.401	20.775		
30	ATOM	2243	CG	GLN			29.408	4.837	22.115	1.00 27.34	A
	ATOM	2244	CD	GLN			29.638	5.914	23.156	1.00 27.19	A
	ATOM	2245		GLN			28.875	6.872	23.252	1.00 28.29	A
	ATOM	2246		GLN			30.687	5.753	23.951	1.00 28.79	A
25	ATOM	2247	С	GLN			28.375	4.989	18.385	1.00 29.00	A
35	ATOM	2248	0	GLN			29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR			27.053	4.984	18.276	1.00 27.31	
	ATOM	2250	CA	THR			26.390	5.568	17.119	1.00 27.85	
	ATOM	2251	СВ	THR			24.991	4.941	16.904	1.00 30.69	A
40	ATOM	2252		THR			25.132	3.532	16.665	1.00 30.07	
40	ATOM	2253		THR			24.289	5.585	15.709	1.00 29.58	A
	ATOM	2254	С	THR			26.244	7.062	17.376	1.00 26.85	A
	ATOM	2255	0	THR			25.592	7.475	18.329	1.00 25.77	A
	ATOM	2256	N	PRO			26.867	7.898	16.533	1.00 27.22	A
	ATOM	2257	CD	PRO			27.792	7.588	15.431	1.00 25.89	A
45	ATOM	2258	CA	PRO			26.763	9.346	16.734	1.00 27.23	A
	ATOM	2259	СВ	PRO			27.625	9.915	15.609	1.00 24.91	A
	ATOM	2260	CG			355	28.643	8.838	15.385	1.00 25.54	A
	ATOM	2261	С			355	25.322	9.837	16.641	1.00 28.07	A
	ATOM	2262	0			355	24.548	9.364	15.810	1.00 27.24	A
50	ATOM	2263	N			356	24.941	10.792	17.500	1.00 28.28	A
	ATOM	2264	CD			356	25.752	11.560	18.462	1.00 28.31	
	ATOM	2265	CA			356	23.572	11.306	17.448	1.00 28.44	A
	ATOM	2266	СВ	PRO			23.539	12.301	18.604	1.00 28.11	A
	ATOM	2267	CG			356	24.946	12.832	18.612	1.00 26.86	A
55	ATOM	2268	С			356	23.363	11.978	16.097	1.00 29.25	A
	ATOM	2269	0	PRO			24.304	12.537	15.529	1.00 27.27	A
	ATOM	2270	N	ALA			22.143	11.910	15.575	1.00 30.45	A
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00 32.81	A
	ATOM	2272	CB	ALA	Α	357	20.507	12.019	13.757	1.00 31.99	A

	ATOM	2273	С	ALA	Α	357	21.824	14.035	14.448	1.00 35.05	A
	ATOM	2274	0	ALA	Δ	357	21.194	14.561	15.369	1.00 35.04	А
	ATOM	2275	Ν	LEU			22.516	14.730	13.552	1.00 37.81	A
	ATOM	2276	CA	LEU	Α	358	22.578	16.185	13.597	1.00 42.15	A
5	ATOM	2277	СВ	LEU	7\	358	23.679	16.681	12.658	1.00 39.54	А
5											
	ATOM	2278	CG	LEU	Α	358	25.086	16.285	13.109	1.00 39.51	A
	ATOM	2279	CD1	LEU	Α	358	26.102	16.686	12.062	1.00 39.29	A
	ATOM	2280		LEU			25.395	16.953	14.445	1.00 40.01	А
	ATOM	2281	С	LEU	Α	358	21.241	16.837	13.242	1.00 45.91	A
10	ATOM	2282	0	LEU	Α	358	20.874	16.927	12.069	1.00 45.71	A
	ATOM	2283	N	THR			20.530	17.290	14.275	1.00 50.06	А
	ATOM	2284	CA	THR	Α	359	19.223	17.939	14.140	1.00 53.73	A
	MOTA	2285	СВ	THR	Α	359	19.353	19.428	13.726	1.00 54.04	A
	ATOM	2286		THR			19.995	19.521	12.448	1.00 56.35	A
15	ATOM	2287	CG2	THR	Α	359	20.158	20.204	14.763	1.00 54.32	A
	ATOM	2288	С	THR	Α	359	18.309	17.236	13.139	1.00 54.47	A
	ATOM	2289	0	THR			18.483	16.016	12.930	1.00 55.90	А
	ATOM	2290	TXO	THR	Α	359	17.407	17.908	12.595	1.00 56.97	A
	ATOM	2291	OH2	TIP	S	1	42.566	19.118	34.302	1.00 15.09	S
20	ATOM	2292		TIP	S	2	41.052	32.378	19.857	1.00 15.82	S
20											
	ATOM	2293	OH2	TIP	S	3	37.014	33.030	17.747	1.00 16.95	S
	ATOM	2294	OH2	TIP	S	5	45.353	24.370	18.152	1.00 16.85	S
	ATOM	2295		TIP	S	6	31.896	13.930	33.235	1.00 20.42	S
	ATOM	2296	OH2		S	7	50.351	22.781	28.249	1.00 21.14	S
25	ATOM	2297	OH2	TIP	S	8	45.246	-0.589	-0.734	1.00 17.74	S
	ATOM	2298	OH2	TIP	S	11	46.249	-0.348	-8.523	1.00 21.32	S
		2299				14	45.756	11.148	29.680	1.00 21.94	S
	ATOM		OH2		S						
	ATOM	2300	OH2	TIP	S	15	44.273	13.157	34.592	1.00 15.61	S
	ATOM	2301	OH2	TIP	S	17	53.598	3.722	-1.720	1.00 21.45	S
30	ATOM	2302	OH2	TIP	S	18	46.049	13.087	31.565	1.00 20.35	S
50											
	ATOM	2303		TIP	S	19	53.422	22.401	-3.280	1.00 23.26	S
	ATOM	2304	OH2	TIP	S	20	34.587	7.922	5.383	1.00 22.58	S
	ATOM	2305	OH2	TIP	S	21	45.053	27.379	19.376	1.00 29.60	S
					S	23				1.00 31.68	S
	ATOM	2306	OH2				28.899	36.416	28.633		
35	ATOM	2307	OH2	TIP	S	24	35.531	11.645	-8.219	1.00 23.45	S
	ATOM	2308	OH2	TIP	S	25	47.364	28.787	19.612	1.00 23.03	S
	ATOM	2309	OH2	TIP	ď	27	48.859	21.588	12.634	1.00 23.76	S
	MOTA	2310	OH2	TIP	S	29	48.805	8.920	23.626	1.00 22.23	S
	ATOM	2311	OH2	TIP	S	31	48.619	7.247	10.112	1.00 21.32	S
40	ATOM	2312	OH2	TIP	S	34	44.824	28.720	15.621	1.00 25.27	S
10				TIP							
	ATOM	2313				35	26.030	12.634	13.407	1.00 21.61	S
	MOTA	2314	OH2	TIP	S	36	50.462	19.810	40.066	1.00 25.45	S
	MOTA	2315	OH2	TIP	S	37	39.631	23.510	-0.239	1.00 30.88	S
	ATOM	2316		TIP		40	44.734	42.655	10.346	1.00 30.84	S
4.5											
45	ATOM	2317	OH2	TIP	S	41	54.653	3.902	1.503	1.00 27.14	S
	ATOM	2318	OH2	TIP	S	45	45.693	21.923	39.754	1.00 28.30	S
	ATOM	2319		TIP		47	47.820	16.413	7.805	1.00 25.73	S
	MOTA	2320		TIP		48	50.292	31.412	29.642	1.00 32.79	S
	ATOM	2321	OH2	TIP	S	49	26.056	16.646	34.827	1.00 29.80	S
50	ATOM	2322	OH2	TIP	S	52	31.714	10.996	31.855	1.00 29.15	S
•											
	ATOM	2323		TIP		53	46.108	23.843	-4.299	1.00 24.21	S
	MOTA	2324	OH2	TIP	S	54	37.645	11.206	34.448	1.00 28.56	S
	ATOM	2325	OH2	TIP	S	55	26.371	28.513	12.142	1.00 32.08	S
								19.700			
	ATOM	2326		TIP		58	33.564		3.483	1.00 28.28	S
55	ATOM	2327		TIP		64	48.295	-0.632	14.280	1.00 32.13	S
	ATOM	2328	OH2	TIP	S	65	40.064	26.036	34.324	1.00 24.17	S
	ATOM	2329		TIP		66	29.570	3.958	14.729	1.00 28.94	S
	ATOM	2330		TIP		72	60.085	11.604	6.814	1.00 38.35	S
	ATOM	2331	OH2	TIP	S	73	39.203	44.403	18.686	1.00 26.61	S

	ATOM	2332	OH2	${\tt TIP}$	S	76	47.312	12.366	27.366	1.00	28.51	S	3
	ATOM	2333	OH2	TIP	S	80	43.862	33.771	33.329	1.00	28.82	S	3
	ATOM	2334		TIP	S	81	57.890	13.106	2.128		40.62	S	
	MOTA	2335	OH2	TIP	S	82	41.663	34.381	32.043	1.00	19.35	S	3
5	ATOM	2336	OH2	TIP	S	85	50.974	40.331	19.200	1.00	21.14	5	3
-	ATOM	2337			S	88	47.925	-0.832	-6.556		24.11	5	
	ATOM	2338	OH2		S	90	27.231	28.336	33.481		27.64	S	
	MOTA	2339	OH2	TIP	S	91	43.651	-7.101	-7.995	1.00	24.33	S	3
	ATOM	2340	OH2	TIP	S	92	49.325	4.387	19.370	1.00	28.02	S	3
10	ATOM	2341		TIP	Q	93	46.231	11.549	33.898		29.40	S	
10													
	ATOM	2342	OH2	TIP	S	94	63.889	24.831	1.168		26.53		3
	ATOM	2343	OH2	TIP	S	96	56.396	4.952	-6.749	1.00	28.00	S	3
	ATOM	2344	OH2	TIP	S	98	35.510	27.986	11.558	1.00	29.24	S	3
	ATOM	2345		TIP			49.942	24.366	30.265		31.61	5	
1.7													
15	ATOM	2346		TIP		101	56.121	7.113	-8.298		31.57	S	
	ATOM	2347	OH2	TIP	S	102	58.318	19.957	-8.378	1.00	26.95	5	3
	ATOM	2348	OH2	TIP	S	103	49.647	22.446	39.624	1.00	40.57	5	3
	ATOM	2349		TIP		104	45.359	7.052	13.052		26.27	S	
	ATOM	2350		TIP			37.150	32.340	32.346		34.45	S	
20	ATOM	2351	OH2	TIP	S	107	43.465	40.457	8.240	1.00	40.48	S	3
	ATOM	2352	OH2	TIP	S	119	36.644	8.257	13.418	1.00	30.70	5	3
	ATOM	2353	OH2	TIP		123	41.912	-8.974	-8.264		26.08	S	
	ATOM	2354		TIP			62.424	15.800	-7.411		24.08	S	
	ATOM	2355	OH2	TIP	S	126	37.266	18.656	-9.097		28.99	S	3
25	ATOM	2356	OH2	TIP	S	127	43.129	26.845	14.606	1.00	25.19	S	3
	ATOM	2357	OH2	TIP	S	128	36.339	32.639	29.802		29.25	S	
									26.498				
	ATOM	2358	OH2	TIP		130	54.051	14.561			33.93	5	
	ATOM	2359	OH2	TIP	S	131	41.805	-4.242	5.492	1.00	33.72	2	
	ATOM	2360	OH2	TIP	S	133	38.873	25.163	36.697	1.00	30.69	S	3
30	ATOM	2361	OH2	TIP	S	134	28.777	8.553	25.307	1.00	31.43	S	3
	ATOM	2362	OH2			135	53.672		-12.803		33.45	5	
	ATOM	2363	OH2	TIP		136	59.892	15.434	11.467		31.39	2	
	ATOM	2364	OH2	TIP	S	137	31.040	12.361	35.470	1.00	34.07	2	3
	ATOM	2365	OH2	TIP	S	139	33.489	14.292	-0.598	1.00	40.68	5	3
35	ATOM	2366	ОН2			140	46.918	8.748	11.662		29.23	2	
33													
	ATOM	2367	OH2			141	46.297	-7.287	-9.196		42.20	2	
	MOTA	2368	OH2	TIP	S	142	58.193	6.715	-4.685	1.00	35.48	S	3
	ATOM	2369	OH2	TIP	S	143	44.598	4.435	12.503	1.00	27.68	5	3
	ATOM	2370	OH2	TIP	S	144	27.003	5.999	12.450	1.00	36.30	S	3
40	ATOM	2371				145	43.676	32.852	35.735		35.70	5	
40													
	ATOM	2372		TIP			35.783	18.628	36.452		34.62	S	
	MOTA	2373	OH2	TIP	S	147	25.402	4.058	20.638	1.00	45.03	S	S
	ATOM	2374	OH2	TIP	S	148	45.839	35.853	33.724	1.00	35.47	5	S
	ATOM	2375		TIP			22.176	18.976	16.752		31.87		3
15													
45	ATOM	2376		TIP			43.986	33.179	10.162		37.70		3
	MOTA	2377	OH2	TIP	S	151	50.653	20.347	42.428	1.00	35.80	S	S
	MOTA	2378	OH2	TIP	S	152	47.843	24.314	9.506	1.00	31.05	S	3
	ATOM	2379		TIP			44.693		-14.175		29.90	S	
	ATOM	2380		TIP			26.560	36.851	31.684		49.29	S	
50	ATOM	2381	OH2	TIP	S	156	46.867	8.019	-12.951	1.00	29.21	S	3
	ATOM	2382	OH2	TIP	S	157	30.432	28.741	12.438	1.00	37.76	S	3
	ATOM	2383		TIP			41.004	20.553	6.423		39.53	S	
	ATOM	2384		TIP			49.258	20.069	29.294		33.97	5	
	ATOM	2385		TIP			48.082	28.459	16.489		33.10		3
55	ATOM	2386	OH2	TIP	S	161	47.448	18.625	27.683	1.00	34.87	S	3
	ATOM	2387	OH2	TIP	S	162	19.687	20.632	23.411	1.00	35.01		3
				TIP			32.402	-1.266			37.26		3
	ATOM	2388							22.443				
	ATOM	2389		TIP			39.475	33.468	33.237		35.34		3
	ATOM	2390	OH2	TIP	S	165	44.277	18.950	5.162	1.00	45.14	S	3

	ATOM	2391	OH2 TIP S	166	34.797	30.523	10.736	1.00 47.55	S
	ATOM	2392	OH2 TIP S	167	46.541	3.526	-14.949	1.00 26.54	S
	ATOM	2393	OH2 TIP S		36.333	16.371	1.539	1.00 38.68	S
	ATOM	2394	OH2 TIP S		46.761	38.936	27.403	1.00 34.66	S
5	MOTA	2395	OH2 TIP S	170	24.163	13.264	11.375	1.00 41.23	S
	ATOM	2396	OH2 TIP S	171	48.459	15.018	31.951	1.00 38.11	S
	ATOM	2397	OH2 TIP S		34.261	23.193	40.004	1.00 48.96	S
		2398	OH2 TIP S		45.924	-0.026	13.224	1.00 39.55	S
	ATOM								
	ATOM	2399	OH2 TIP S		41.384	37.389	32.543	1.00 40.74	S
10	MOTA	2400	OH2 TIP S	177	49.394	35.312	27.150	1.00 44.33	S
	MOTA	2401	OH2 TIP S	178	29.066	29.942	34.359	1.00 41.46	S
	ATOM	2402	OH2 TIP S	180	49.354	19.467	7.273	1.00 34.56	S
	ATOM	2403	OH2 TIP S		25.298	17.029	31.863	1.00 47.74	S
		2403	OH2 TIP S					1.00 47.74	S
1.5	ATOM				37.071	25.027	4.669		
15	ATOM	2405	OH2 TIP S		22.581	7.487	18.691	1.00 41.75	S
	ATOM	2406	OH2 TIP S	184	32.269	7.011	-1.891	1.00 48.84	S
	ATOM	2407	OH2 TIP S	185	48.234	0.494	6.833	1.00 48.16	S
	ATOM	2408	OH2 TIP S	187	20.008	14.658	19.211	1.00 45.27	S
	ATOM	2409	OH2 TIP S		49.341	22.698	42.272	1.00 42.20	S
20									
20	ATOM	2410	OH2 TIP S		61.292	18.260	-8.097	1.00 45.21	S
	MOTA	2411	OH2 TIP S	191	28.152	10.606	2.819	1.00 40.38	S
	MOTA	2412	OH2 TIP S	192	25.626	12.619	23.191	1.00 34.27	S
	ATOM	2413	OH2 TIP S	193	59.876	11.603	1.216	1.00 46.54	S
	ATOM	2414	OH2 TIP S		57.592		-10.646	1.00 45.82	S
25	ATOM	2415		195	31.509	36.649	21.499	1.00 38.73	S
23									
	ATOM	2416	OH2 TIP S		50.270	-1.543	-6.136	1.00 42.66	S
	MOTA	2417	OH2 TIP S	198	24.467	8.729	13.088	1.00 42.78	S
	MOTA	2418	OH2 TIP S	199	38.098	8.699	25.759	1.00 32.80	S
	ATOM	2419	OH2 TIP S	200	57.831	11.358	-13.255	1.00 45.31	S
30	ATOM	2420	OH2 TIP S		23.888	22.328	30.524	1.00 37.12	S
50	ATOM	2421	OH2 TIP S		47.691	26.068	37.666	1.00 37.92	S
	ATOM	2422	OH2 TIP S		38.653	7.070	29.307	1.00 50.54	S
	MOTA	2423	OH2 TIP S	206	44.424	27.583	2.092	1.00 53.50	S
	MOTA	2424	OH2 TIP S	212	22.258	2.296	17.948	1.00 47.38	S
35	ATOM	2425	OH2 TIP S	214	19.843	17.943	23.303	1.00 30.36	S
	ATOM	2426		216	27.647	11.344	24.681	1.00 31.32	S
	ATOM	2427	OH2 TIP S		37.953	7.817	-9.284	1.00 45.97	S
	ATOM	2428	OH2 TIP S		33.845	34.040	12.124	1.00 38.11	S
	MOTA	2429	OH2 TIP S		58.484	15.269	13.717	1.00 38.26	S
40	ATOM	2430	OH2 TIP S	220	48.526	40.920	26.583	1.00 35.23	S
	ATOM	2431	OH2 TIP S	222	52.094	21.184	38.122	1.00 29.86	S
	ATOM	2432	OH2 TIP S		36.889	5.881	3.281	1.00 37.63	S
	ATOM	2433	OH2 TIP S		47.642		-10.684	1.00 34.89	S
	MOTA	2434	OH2 TIP S		47.284	2.916		1.00 34.10	S
45	ATOM	2435	OH2 TIP S		42.468		-15.039	1.00 37.98	S
	MOTA	2436	OH2 TIP S	228	19.169	22.832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S	231	57.592	12.689	14.880	1.00 50.22	S
	ATOM	2438	OH2 TIP S		27.102	9.176	5.655	1.00 40.57	S
	ATOM	2439	OH2 TIP S		58.618		-11.925	1.00 50.71	S
50									
50	ATOM	2440	OH2 TIP S		22.822	25.342	19.945	1.00 34.93	S
	ATOM	2441	OH2 TIP S	236	24.831	32.218	28.901	1.00 37.69	S
	MOTA	2442	OH2 TIP S	237	20.045	10.774	16.992	1.00 39.57	S
	ATOM	2443	OH2 TIP S	238	58.019	19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S		19.490	20.949	26.114	1.00 34.55	S
55			OH2 TIP S						S
ננ	ATOM	2445			61.187	26.377	7.346	1.00 39.68	
	ATOM	2446	OH2 TIP S		33.680	38.342	19.389	1.00 48.93	S
	MOTA	2447	OH2 TIP S		51.539	31.612	10.881	1.00 55.65	S
	ATOM	2448	OH2 TIP S	244	25.872	14.431	30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP S		37.332	5.849	9.544	1.00 43.81	S

	ATOM	2450	OH2	TIP	S 25	0	39.087	-1.293	-9.655	1.00	42.96	S
	ATOM	2451	OH2	ΤΤΡ	s 25	8	23.938	30.000	30.010	1.00	38.89	S
	ATOM	2452			s 25		24.949	29.749	32.578		40.17	S
	ATOM	2453			S 26		32.111	17.986	1.918		48.36	S
5	MOTA	2454	OH2	TIP	S 26	6	21.404	12.876	25.603	1.00	57.17	S
	ATOM	2455	OH2	TIP	s 26	9	35.425	36.767	12.550	1.00	30.70	S
	ATOM	2456	ОН2	TIP	s 27	Λ	52.438	25.529	30.131	1 00	44.85	S
				TIP			53.299	20.156			37.15	S
	ATOM	2457							36.003			
	ATOM	2458			S 27		50.914	6.919	23.723		43.29	S
10	MOTA	2459	OH2	TIP	S 27	4	31.578	30.795	11.014	1.00	50.15	S
	MOTA	2460	OH2	TIP	s 27	5	26.341	7.243	22.447	1.00	39.40	S
	ATOM	2461	OH2	TIP	s 27	6	60.392	18.195	10.235	1.00	37.91	S
	ATOM	2462	OH2				47.355		-10.821		48.18	S
					S 27		41.304		-16.647		38.12	S
1.7	ATOM	2463										
15	ATOM	2464			S 28		33.299	21.620	37.881		46.29	S
	ATOM	2465	OH2	TIP	S 28	3	56.469	26.112	-8.575	1.00	43.71	S
	ATOM	2466	OH2	TIP	S 28	7	48.382	26.573	7.246	1.00	41.43	S
	ATOM	2467	OH2	ΤΤΡ	S 28	8	56.240		-11.331	1.00	41.79	S
	ATOM	2468			S 29		49.060	14.978	28.166		37.03	S
20												
20	ATOM	2469			S 29		37.095	44.270	26.442		45.08	S
	MOTA	2470			S 29		47.814	-0.384	-13.299	1.00	48.60	S
	MOTA	2471	OH2	TIP	S 29	7	58.081	2.784	-7.841	1.00	41.89	S
	ATOM	2472	OH2	TIP	S 29	8	36.447	45.321	18.644	1.00	54.91	S
	ATOM	2473			s 29		49.029	23.328	1.767		30.55	S
25	ATOM	2474			S 30		24.375	13.771	8.634		48.47	S
23												
	ATOM	2475		TIP			47.904	36.798	28.653		35.76	S
	MOTA	2476	OH2	TIP	S 30	5	51.156	40.821	27.172	1.00	43.59	S
	MOTA	2477	OH2	TIP	S 30	6	32.943	28.917	35.227	1.00	42.60	S
	ATOM	2478	OH2	TIP	s 30	7	58.462	28.373	6.251	1.00	46.15	S
30	ATOM	2479		TIP			41.964	30.940	36.712		48.26	S
50	ATOM	2480			S 31		51.176	-1.922	-3.336		50.61	S
	ATOM	2481			S100		21.319	36.868	23.805		36.97	S
	MOTA	2482	OH2	TIP	S100	2	48.880	32.620	27.617	1.00	44.40	S
	MOTA	2483	OH2	TIP	S100	3	61.880	19.473	11.767	1.00	45.49	S
35	ATOM	2484	OH2	TIP	S100	4	52.770	21.424	26.815	1.00	24.43	S
	ATOM	2485			S100		35.373	29.094	36.197		35.97	S
	ATOM	2486			S100		40.815	-6.636	4.389		43.15	S
	ATOM	2487			S100		44.953	1.286	11.272		49.45	S
	ATOM	2488			S101		21.004	16.168	27.009	1.00	48.51	S
40	MOTA	2489	OH2	TIP	S101	.1	47.094	41.786	9.243	1.00	50.10	S
	ATOM	2490	OH2	TIP	S101	.2	32.479	2.978	14.158	1.00	49.47	S
	ATOM	2491	012	GLC	G	1	48.557	11.372	-12.279	1.00	40.72	G
	ATOM	2492	C11			1	48.836		-11.097		38.05	G
	ATOM	2493	C13			1	49.266		-11.476		38.09	G
4.5												
45	ATOM	2494	014			1	49.559		-10.292		33.99	G
	MOTA	2495	C15	GLC	G	1	48.150	14.257	-12.257	1.00	37.32	G
	ATOM	2496	016	GLC	G	1	48.574	15.582	-12.604	1.00	36.74	G
	ATOM	2497	012	GLC	G	2	40.114	-6.634	-6.562	1.00	33.52	G
	ATOM	2498	C11			2	38.967	-6.592	-7.404		31.05	G
50			C13					-6.417				
30	ATOM	2499				2	37.712		-6.552		31.56	G
	ATOM	2500	014			2	36.554	-6.406	-7.389		30.70	G
	MOTA	2501	C15	GLC	G	2	37.792	-5.109	-5.761	1.00	30.03	G
	MOTA	2502	016	GLC	G	2	36.609	-4.961	-4.975	1.00	29.66	G
	ATOM	2503	012	GLC	G	3	44.030	8.243	-13.470	1.00	37.90	G
55	ATOM	2504	C11			3	43.950		-13.690		38.47	G
22												
	ATOM	2505	C13			3	42.747		-14.579		39.52	G
	ATOM	2506	014			3	41.551		-13.942		39.39	G
	ATOM	2507	C15			3	42.878	9.280	-15.934		41.43	G
	ATOM	2508	016	GLC	G	3	41.736	9.613	-16.731	1.00	40.78	G

	ATOM	2509	012	GLC	G	5	40.556	1.005	2.289	1.00	45.25	G
	ATOM	2510		GLC		5	40.966	2.332	1.960		40.56	G
	ATOM	2511		GLC		5	40.187	3.327	2.814		40.36	Ğ
	ATOM	2512		GLC		5	38.791	3.169	2.572		40.71	G
-												
5	ATOM	2513		GLC		5	40.619	4.751	2.464		40.04	G
	ATOM	2514		GLC		5	39.885	5.681	3.256		36.89	G
	ATOM	2515		GLC		6	36.951	22.702	40.046		63.04	G
	MOTA	2516	C11	GLC	G	6	37.592	21.583	39.422	1.00	62.46	G
	MOTA	2517	C13	GLC	G	6	38.104	21.978	38.030	1.00	61.14	G
10	ATOM	2518	014	GLC	G	6	39.034	23.054	38.168	1.00	61.72	G
	ATOM	2519	C15	GLC	G	6	36.948	22.429	37.126	1.00	60.51	G
	ATOM	2520	016	GLC	G	6	35.992	21.372	36.960	1.00	58.61	G
	ATOM	2521		GLC		7	37.316	0.281	14.299		73.45	G
	ATOM	2522		GLC		7	37.655	-0.758	15.222		72.78	G
15	ATOM	2523		GLC		7	36.592	-1.856	15.157		72.78	G
13		2524		GLC		7	35.320	-1.299	15.137		73.88	G
	ATOM											
	ATOM	2525		GLC		7	36.924	-2.989	16.134		73.66	G
	ATOM	2526		GLC		7	36.972	-2.493	17.478		75.38	G
	ATOM	2527		GLC		8	51.921	21.898	5.908		62.51	G
20	ATOM	2528	C11	GLC	G	8	52.447	20.871	5.063	1.00	63.42	G
	ATOM	2529	C13	GLC	G	8	51.476	20.597	3.908	1.00	64.28	G
	MOTA	2530	014	GLC	G	8	51.297	21.794	3.150	1.00	66.28	G
	ATOM	2531	C15	GLC	G	8	50.121	20.137	4.448	1.00	64.49	G
	ATOM	2532	016	GLC	G	8	49.233	19.886	3.357	1.00	64.01	G
25	ATOM	2533	012	GLC	G	10	36.044	37.499	29.523	1.00	56.89	G
	ATOM	2534		GLC		10	35.164	36.645	30.259		56.97	G
	ATOM	2535		GLC		10	33.849	36.489	29.494		56.11	G
	ATOM	2536		GLC		10	33.248	37.772	29.308		56.44	G
	ATOM	2537		GLC		10	32.900	35.580	30.277		55.84	G
30	ATOM	2538		GLC		10	31.674	35.442	29.557		55.39	G
30		2539		ATP		1		25.658				
	ATOM						46.280		5.170		51.49	N
	ATOM	2540	PG	ATP		1	46.464	25.053	3.691		52.22	N
	ATOM	2541		ATP		1	47.406	23.911	3.763		51.41	N
	ATOM	2542		ATP		1	46.794	26.182	2.784		52.07	N
35	ATOM	2543	03B	ATP		1	44.976	24.513	3.344		51.01	N
	MOTA	2544	PB	ATP	Ν	1	44.560	22.969	3.605	1.00	50.20	N
	MOTA	2545	01B	ATP	N	1	43.083	22.898	3.669	1.00	49.41	N
	MOTA	2546	02B	ATP	N	1	45.345	22.474	4.766	1.00	50.34	N
	ATOM	2547	03A	ATP	N	1	45.070	22.231	2.255	1.00	47.77	N
40	ATOM	2548	PA	ATP	N	1	45.075	20.613	2.121	1.00	42.84	N
	ATOM	2549	01A	ATP		1	45.547	20.291	0.754		43.81	N
	ATOM	2550		ATP		1	45.807	20.035	3.270		45.03	N
	ATOM	2551		ATP		1	43.516	20.223	2.245		41.73	N
	ATOM	2552		ATP		1	42.528	20.925	1.489		37.57	N
45	ATOM	2553		ATP		1	41.127	20.379	1.776		39.45	N
7.7												
	ATOM	2554		ATP		1	40.907	19.024	1.279		37.72	N
	ATOM	2555		ATP		1	40.777	20.321	3.251		38.48	N
	ATOM	2556		ATP		1	40.360	21.615	3.697		40.42	N
	ATOM	2557		ATP		1	39.608	19.374	3.270		37.58	N
50	ATOM	2558		ATP		1	38.410	20.076	2.924		35.98	N
	MOTA	2559	C1*	ATP	N	1	39.939	18.346	2.173		35.55	N
	ATOM	2560	N9	ATP	N	1	40.628	17.156	2.747	1.00	31.76	N
	ATOM	2561	C8	ATP	N	1	41.864	17.126	3.274	1.00	30.49	N
	ATOM	2562	N7	ATP	N	1	42.143	15.877	3.667	1.00	29.75	N
55	ATOM	2563	С5	ATP		1	41.088	15.118	3.390		27.49	N
	ATOM	2564	C4	ATP		1	40.125	15.925	2.810		30.02	N
	ATOM	2565	N3	ATP		1	38.937	15.389	2.431		27.11	N
	ATOM	2566	C2	ATP		1	38.679	14.085	2.615		25.62	N
	ATOM	2567	N1	ATP		1	39.597	13.283	3.175		21.76	N
	AION	2001	TA T	VIL	ΤΛ	Т	JJ.JJ/	10.403	J. I / J	1.00	21./0	IN

	ATOM	2568	С6	ATP	N	1	40.800	13.768	3.571	1.00 23.	.90 N
	MOTA	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00 21.	.94 N
	MOTA	2570	S	SO4	I	1	58.680	8.493	-0.639	1.00 56.	.05 I
	MOTA	2571	01	SO4	I	1	57.956	7.875	0.483	1.00 58.	.83 I
5	MOTA	2572	02	SO4	I	1	57.886	9.607	-1.188	1.00 57.	.04 I
	MOTA	2573	03	SO4	I	1	58.906	7.478	-1.683	1.00 57.	.47 I
	MOTA	2574	04	SO4	I	1	59.976	9.008	-0.156	1.00 57.	.51 I
	MOTA	2575	S	SO4	I	2	39.339	4.855	7.057	1.00 84.	.24 I
	MOTA	2576	01	SO4	I	2	39.390	6.175	7.711	1.00 85.	.02 I
10	ATOM	2577	02	SO4	Ι	2	40.101	4.897	5.797	1.00 84.	.75 I
	MOTA	2578	03	SO4	Ι	2	37.936	4.506	6.766	1.00 84.	.94 I
	ATOM	2579	04	SO4	I	2	39.931	3.842	7.954	1.00 84.	.44 I
	MOTA	2580	S	SO4	I	3	38.987	-2.256	3.310	1.00 58.	.58 I
	MOTA	2581	01	SO4	I	3	37.734	-1.675	3.827	1.00 59.	.11 I
15	ATOM	2582	02	SO4	I	3	39.460	-1.454	2.172	1.00 59.	
	ATOM	2583	03	SO4	I	3	38.743	-3.640	2.866	1.00 60.	.97 I
	ATOM	2584	04	SO4	I	3	40.014	-2.260	4.369	1.00 59.	.58 I
	MOTA	2585	S	SO4	I	4	34.397	5.289	30.981	1.00 64.	.34 I
	ATOM	2586	01	SO4	I	4	33.627	6.528	30.742	1.00 60.	
20	ATOM	2587	02	SO4	I	4	34.337	4.427	29.782	1.00 60.	.11 I
	ATOM	2588	03	SO4	Ι	4	33.816	4.572	32.133	1.00 64.	.39 I
	ATOM	2589	04	SO4	Ι	4	35.806	5.626	31.277	1.00 63.	
	ATOM	2590	S	SO4	I	5	55.074	-6.984	-3.711	1.00 75.	.40 I
	MOTA	2591	01	SO4	Ι	5	54.657	-7.518	-2.399	1.00 74.	.66 I
25	MOTA	2592	02	SO4	Ι	5	54.209	-5.845	-4.065	1.00 74.	.96 I
	ATOM	2593	03	SO4	I	5	54.950	-8.034	-4.742	1.00 74.	.22 I
	MOTA	2594	04	SO4	Ι	5	56.477	-6.532	-3.633	1.00 75.	
	MOTA	2595	02	PO4	Ρ	100	57.362	24.998	13.149	1.00 66.	.76 P
	ATOM	2596	03	PO4	Ρ	100	59.399	26.166	13.761	1.00 66.	
30	ATOM	2597	04	PO4	Ρ	100	57.761	25.606	15.462	1.00 67.	
	ATOM	2598	01	PO4	Ρ	100	57.264	27.325	13.818	1.00 65.	
	ATOM	2599	P	PO4	Ρ	100	57.947	26.025	14.048	1.00 66.	.69 P
	END										

Example 4: Co-ordinates for the dimer of the PDK1 fragment, without alternate side chains. Chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

	ATOM	1	СВ	PRO A	71	58.912	-7.251	8.216	1.00 6	7.78	А
40	ATOM	2	CG	PRO A	71	59.621	-6.941	9.534	1.00 6	9.16	A
	ATOM	3	С	PRO A	71	59.493	-6.506	5.894	1.00 6	7.06	A
	ATOM	4	0	PRO A	71	59.196	-5.318	5.766	1.00 6	6.66	A
	ATOM	5	N	PRO A	71	60.984	-6.073	7.833	1.00 6	7.86	A
	ATOM	6	CD	PRO A	71	60.554	-5.762	9.207	1.00 6	8.24	A
45	ATOM	7	CA	PRO A	71	60.040	-7.035	7.217	1.00 6	7.75	A
	ATOM	8	N	PRO A	72	59.356	-7.385	4.890	1.00 6	6.32	A
	ATOM	9	CD	PRO A	72	59.712	-8.816	4.898	1.00 6	7.17	A
	ATOM	10	CA	PRO A	72	58.840	-6.986	3.578	1.00 6	5.61	A
	ATOM	11	СВ	PRO A	72	58.672	-8.321	2.858	1.00 6	6.47	A
50	ATOM	12	CG	PRO A	72	59.796	-9.133	3.419	1.00 6	7.57	A
	ATOM	13	С	PRO A	72	57.527	-6.208	3.673	1.00 6	3.94	A
	ATOM	14	0	PRO A	72	56.710	-6.451	4.561	1.00 6	4.11	A
	ATOM	15	N	ALA A	73	57.341	-5.268	2.753	1.00 6	1.57	A
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708	1.00 5	8.74	A
55	ATOM	17	СВ	ALA A	73	56.438	-3.030	3.165	1.00 5	8.05	А

	ATOM	18	С	ALA	7\	73	55.626	-4.448	1.271	1.00 56.78	А
	ATOM	19	0	ALA		73	56.347	-4.834	0.349	1.00 56.95	
											A
	MOTA	20	N	PRO		74	54.372	-4.024	1.057	1.00 54.15	A
_	ATOM	21	CD	PRO		74	53.335	-3.610	2.018	1.00 53.31	A
5	ATOM	22	CA	PRO		74	53.856	-4.003	-0.314	1.00 52.54	A
	ATOM	23	СВ	PRO		74	52.474	-3.375	-0.148	1.00 52.86	A
	ATOM	24	CG	PRO	Α	74	52.067	-3.824	1.226	1.00 52.88	A
	ATOM	25	С	PRO	A	74	54.772	-3.167	-1.204	1.00 50.08	A
	ATOM	26	0	PRO	Α	74	55.559	-2.361	-0.708	1.00 49.96	A
10	ATOM	27	N	ALA	А	75	54.680	-3.366	-2.514	1.00 47.58	А
	ATOM	28	CA	ALA	Α	75	55.503	-2.602	-3.446	1.00 44.69	A
	ATOM	29	СВ	ALA	А	75	55.312	-3.121	-4.870	1.00 46.14	А
	ATOM	30	С	ALA		75	55.100	-1.134	-3.371	1.00 41.55	А
	ATOM	31	0	ALA	А	75	53.947	-0.813	-3.086	1.00 41.01	А
15	ATOM	32	N	LYS		76	56.053	-0.245	-3.619	1.00 38.31	A
15	ATOM	33	CA	LYS		76	55.781	1.184	-3.588	1.00 35.72	A
	ATOM	34	CB	LYS		76	57.053	1.957	-3.930	1.00 37.70	A
	ATOM	35	CG	LYS		76	57.123	3.356	-3.350	1.00 40.99	A
		36				76 76	57.262	3.316	-1.836	1.00 40.99	
20	ATOM	36 37	CD	LYS						1.00 40.04	A
20	ATOM		CE	LYS		76 76	57.511	4.705	-1.277		A
	ATOM	38	NΖ	LYS		76	57.681	4.695	0.202	1.00 42.99	A
	ATOM	39	С	LYS		76	54.708	1.467	-4.638	1.00 32.65	A
	ATOM	40	0	LYS		76	54.814	1.005	-5.770	1.00 31.41	A
	ATOM	41	N	LYS		77	53.668	2.207	-4.270	1.00 28.59	A
25	ATOM	42	CA	LYS		77	52.619	2.517	-5.232	1.00 25.72	A
	ATOM	43	СВ	LYS		77	51.316	2.865	-4.509	1.00 26.22	A
	ATOM	44	CG	LYS	Α	77	50.796	1.731	-3.631	1.00 27.15	A
	ATOM	45	CD	LYS	Α	77	49.487	2.089	-2.967	1.00 26.80	A
	ATOM	46	CE	LYS	Α	77	49.136	1.091	-1.870	1.00 27.31	A
30	ATOM	47	NZ	LYS	Α	77	48.998	-0.296	-2.380	1.00 27.17	A
	ATOM	48	С	LYS	Α	77	53.053	3.668	-6.137	1.00 24.67	A
	ATOM	49	0	LYS	Α	77	54.010	4.377	-5.829	1.00 21.60	А
	ATOM	50	N	ARG	Α	78	52.351	3.838	-7.254	1.00 23.66	А
	ATOM	51	CA	ARG	Α	78	52.662	4.897	-8.211	1.00 26.14	A
35	ATOM	52	СВ	ARG		78	53.574	4.344	-9.318	1.00 28.57	A
	ATOM	53	CG	ARG		78	53.017		-10.050	1.00 34.78	A
	ATOM	54	CD	ARG		78	54.092		-10.896	1.00 40.96	A
	ATOM	55	NE	ARG		78	53.560		-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG		78	52.985		-11.203	1.00 52.58	A
40	ATOM	57		ARG		78	52.860	0.113	-9.889	1.00 54.60	A
40	ATOM	58		ARG		78	52.530		-12.022	1.00 54.09	A
	ATOM	59	C	ARG		78	51.382	5.488	-8.803	1.00 23.76	A
			_				50.311				
	MOTA	60	O NT	ARG		78 70		4.888	-8.706	1.00 24.25 1.00 21.76	A
15	ATOM	61	N	PRO		79 70	51.475	6.676	-9.428		A
45	ATOM	62	CD	PRO		79	52.691	7.475	-9.668	1.00 20.82	A
	ATOM	63	CA	PRO		79	50.301		-10.021	1.00 21.96	A
	ATOM	64	СВ	PRO		79	50.910		-10.816	1.00 22.27	A
	ATOM	65	CG	PRO		79	52.124		-10.014	1.00 22.12	A
	ATOM	66	С	PRO		79	49.446		-10.903	1.00 22.86	A
50	ATOM	67	0	PRO		79	48.213		-10.842	1.00 20.52	A
	MOTA	68	N	GLU	Α	80	50.103	5.586	-11.714	1.00 21.87	A
	ATOM	69	CA	GLU	Α	80	49.403	4.685	-12.628	1.00 22.99	A
	ATOM	70	СВ	GLU	Α	80	50.393	3.994	-13.571	1.00 25.24	A
	ATOM	71	CG	GLU	Α	80	51.230	2.907	-12.925	1.00 28.75	A
55	ATOM	72	CD	GLU	Α	80	52.157	2.224	-13.913	1.00 31.99	А
	ATOM	73	OE1	GLU	Α	80	53.072		-14.433	1.00 34.34	А
	ATOM	74		GLU		80	51.969		-14.172	1.00 32.83	А
	ATOM	75	C	GLU		80	48.556		-11.912	1.00 22.09	A
	ATOM	76	0	GLU		80	47.692		-12.530	1.00 22.37	A
		-			-						

	ATOM	77	N	ASP	A	81	48.804	3.413	-10.622	1.00 19.97	A
	ATOM	78	CA	ASP	7\	81	48.026	2.423	-9.874	1.00 19.93	A
	ATOM	79	СВ	ASP		81	48.736	2.029	-8.571	1.00 21.19	A
	MOTA	80	CG	ASP	Α	81	50.089	1.380	-8.807	1.00 22.46	A
5	ATOM	81	OD 1	ASP	Z \	81	50.195	0.554	-9.731	1.00 24.22	A
J											
	ATOM	82	ODZ	ASP		81	51.043	1.685	-8.058	1.00 23.33	A
	ATOM	83	С	ASP	Α	81	46.652	2.975	-9.518	1.00 20.85	A
	ATOM	84	0	ASP	Α	81	45.793	2.246	-9.015	1.00 19.96	A
	ATOM	85	N	PHE		82	46.445	4.258	-9.804	1.00 18.91	A
10											
10	ATOM	86	CA	PHE	А	82	45.200	4.934	-9.465	1.00 19.30	A
	ATOM	87	CB	PHE	Α	82	45.475	6.027	-8.427	1.00 18.43	A
	ATOM	88	CG	PHE	А	82	46.134	5.531	-7.175	1.00 18.01	А
	ATOM	89		PHE		82	45.371	5.136	-6.084	1.00 17.19	A
	ATOM	90		PHE		82	47.520	5.460	-7.086	1.00 18.99	A
15	ATOM	91	CE1	PHE	Α	82	45.977	4.676	-4.918	1.00 17.12	A
	ATOM	92	CE2	PHE	Α	82	48.137	5.000	-5.925	1.00 19.64	А
	ATOM	93	CZ	PHE		82	47.361	4.607	-4.838	1.00 18.00	A
	ATOM	94	С	$_{ m PHE}$	Α	82	44.476	5.596	-10.621	1.00 20.81	A
	ATOM	95	0	PHE	Α	82	45.066	5.933	-11.649	1.00 20.34	A
20	ATOM	96	N	LYS	Δ	83	43.182	5.792	-10.411	1.00 19.80	А
20											
	ATOM	97	CA	LYS		83	42.321		-11.353	1.00 21.65	A
	ATOM	98	СВ	LYS	Α	83	41.096	5.625	-11.687	1.00 22.02	A
	ATOM	99	CG	LYS	Α	83	40.062	6.326	-12.550	1.00 28.93	A
	ATOM	100	CD	LYS		83	38.974		-12.981	1.00 34.20	А
25											
25	ATOM	101	CE	LYS		83	37.909		-13.824	1.00 38.10	A
	ATOM	102	NZ	LYS	Α	83	37.179	7.086	-13.043	1.00 43.33	A
	ATOM	103	С	LYS	Α	83	41.913	7.702	-10.541	1.00 20.74	A
	ATOM	104	0	LYS		83	41.084	7.606	-9.635	1.00 20.98	A
	ATOM	105	N	PHE		8 4	42.513		-10.835	1.00 19.99	A
30	ATOM	106	ca	PHE	Α	84	42.188	10.049	-10.083	1.00 18.63	A
	ATOM	107	СВ	PHE	Δ	84	43.279	11.103	-10.258	1.00 18.95	А
		108	CG	PHE		84	44.571	10.741	-9.587	1.00 17.68	A
	ATOM										
	ATOM	109	CDI	PHE	Α	8 4	45.498	9.926	-10.224	1.00 18.16	A
	ATOM	110	CD2	PHE	A	84	44.843	11.183	-8.299	1.00 19.66	A
35	ATOM	111	CE1	PHE	Δ	8 4	46.676	9.556	-9.589	1.00 18.09	A
		112		PHE		84		10.816	-7.653	1.00 18.89	
	ATOM						46.021				A
	ATOM	113	CZ	PHE	Α	84	46.936	10.002	-8.301	1.00 17.33	A
	ATOM	114	С	PHE	A	84	40.834	10.617	-10.460	1.00 19.69	A
	ATOM	115	0	PHE		8 4	40.391	10 489	-11.601	1.00 20.72	A
40						85					
40	ATOM	116	N	GLY			40.178	11.233	-9.484	1.00 16.80	А
	MOTA	117	CA	$\operatorname{GL} Y$	Α	85	38.872	11.810	-9.716	1.00 17.73	A
	ATOM	118	С	GLY	A	85	38.819	13.280	-9.346	1.00 18.75	A
	ATOM	119	0	GLY	Δ	85	39.740	14.043	-9.650	1.00 18.45	А
	ATOM	120	N	LYS		86	37.753	13.673	-8.659	1.00 16.00	A
45	ATOM	121	CA	LYS	Α	86	37.571	15.064	-8.278	1.00 18.26	A
	ATOM	122	СВ	LYS	Α	86	36.133	15.302	-7.812	1.00 19.00	A
	ATOM	123	CG	LYS		86	35.793	14.660	-6.481	1.00 21.55	A
	ATOM	124	CD	LYS		86	34.368	14.981	-6.066	1.00 26.48	A
	ATOM	125	CE	LYS	Α	86	33.994	14.239	-4.793	1.00 31.92	A
50	ATOM	126	NZ	LYS	А	86	32.568	14.457	-4.412	1.00 35.36	А
	ATOM					86					
		127	С	LYS			38.523	15.571	-7.202	1.00 18.57	A
	ATOM	128	0	LYS		86	39.045	14.807	-6.385	1.00 16.77	A
	ATOM	129	N	ILE	Α	87	38.737	16.881	-7.227	1.00 17.88	A
	ATOM	130	CA	ILE		87	39.577	17.554	-6.256	1.00 18.26	А
55											
55	ATOM	131	СВ	ILE		87	39.994	18.952	-6.772	1.00 19.60	A
	ATOM	132		ILE		87	40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133	CG1	ILE	Α	87	40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134		ILE		87	41.412	20.087	-8.588	1.00 25.26	А
	ATOM	135	С	ILE	Α	87	38.731	17.709	-4.997	1.00 19.67	A

	ATOM	136	0	ILE A	87	37.628	18.249	-5.052	1.00 20.41	А
	ATOM	137	N	LEU A	88	39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU A	88	38.508	17.324	-2.611	1.00 20.68	A
	ATOM	139	СВ	LEU A	88	38.870	16.151	-1.700	1.00 19.97	A
5	ATOM	140	CG	LEU A	88	38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141	CD1	LEU A	88	39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142		LEU A	88	37.029	14.622	-2.359	1.00 18.84	А
	ATOM	143	С	LEU A	88	38.815	18.632	-1.901	1.00 23.11	А
	ATOM	144	0	LEU A	88	37.999	19.146	-1.139	1.00 25.10	A
10	ATOM	145	N	GLY A	89	39.997	19.174	-2.149	1.00 24.09	A
10	ATOM	146	CA	GLY A	89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	C	GLY A	89	41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0	GLY A	89	42.445	20.202	-2.666	1.00 23.47	A
	ATOM	149	N	GLU A	90	41.870	22.254	-1.906	1.00 26.22	A
15		150		GLU A	90	43.064	22.234	-2.404	1.00 28.22	A
13	ATOM		CA							
	ATOM	151	CB	GLU A	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU A	90	42.267	23.038	-4.831	1.00 34.32	A
	ATOM	153	CD	GLU A	90	41.711	23.930	-5.927	1.00 38.27	A
20	ATOM	154		GLU A	90	40.590	24.456	-5.764	1.00 40.57	A
20	ATOM	155		GLU A	90	42.398	24.110	-6.952	1.00 40.90	A
	ATOM	156	С	GLU A	90	43.711	23.768	-1.313	1.00 30.68	A
	MOTA	157	0	GLU A	90	43.049	24.574	-0.668	1.00 32.83	А
	ATOM	158	N	GLY A	91	45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY A	91	45.724	24.332	-0.104	1.00 29.40	A
25	ATOM	160	С	GLY A	91	46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY A	91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER A	92	47.605	25.870	-0.029	1.00 28.30	A
	ATOM	163	CA	SER A	92	48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	СВ	SER A	92	49.165	27.717	0.370	1.00 32.43	A
30	ATOM	165	OG	SER A	92	49.520	27.099	1.593	1.00 40.94	A
	ATOM	166	С	SER A	92	49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER A	92	50.456	26.221	-2.143	1.00 30.46	A
	ATOM	168	N	PHE A	93	50.087	24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE A	93	51.185	23.855	-0.995	1.00 26.34	A
35	ATOM	170	СВ	PHE A	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE A	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE A	93	52.283	25.909	1.392	1.00 29.96	A
	ATOM	173		PHE A	93	53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174	CE1	PHE A	93	52.779	27.181	1.665	1.00 32.69	A
40	ATOM	175		PHE A	93	54.452	26.883	-0.044	1.00 32.63	А
	ATOM	176	CZ	PHE A	93	53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	С	PHE A	93	50.759	22.445	-1.365	1.00 25.39	А
	ATOM	178	0	PHE A	93	51.601	21.559	-1.522	1.00 24.59	А
	ATOM	179	N	SER A	94	49.457	22.235	-1.519	1.00 23.63	А
45	ATOM	180	CA	SER A	94	48.965	20.912	-1.860	1.00 21.43	А
	ATOM	181	СВ	SER A	94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER A	94	48.091	20.475	0.340	1.00 21.19	A
	ATOM	183	C	SER A	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER A	94	46.795	21.882	-2.173	1.00 18.76	A
50	ATOM	185	N	THR A	95	47.174	19.832	-3.038	1.00 19.38	A
30	ATOM	186	CA	THR A	95	45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	CB	THR A	95	45.818	19.818	-5.110	1.00 17.30	A
		188		THR A	95	46.196		-5.434	1.00 22.04	
	ATOM ATOM	189		THR A	95	44.421	21.162 19.549	-5.434 -5.661	1.00 22.04	A n
55										A
55	ATOM	190	C	THR A	95 95	45.455	18.201	-3.243	1.00 18.61	A 7
	ATOM	191	O NI	THR A	95 96	46.212	17.264	-3.524	1.00 17.10	A 7
	MOTA	192	N	VAL A	96	44.295	18.024	-2.623	1.00 16.53	A
	ATOM	193	CA	VAL A	96	43.845	16.685	-2.266	1.00 16.05	A
	ATOM	194	СВ	VAL A	96	43.170	16.672	-0.886	1.00 16.32	A

	ATOM	195	CG1	VAL	Α	96	42.741	15.249	-0.532	1.00	18.02	A
	ATOM	196	CG2	VAL	Δ	96	44.145	17.206	0.168	1.00	16 69	А
	MOTA	197	С	VAL	Α	96	42.875	16.207	-3.335	1.00		A
	ATOM	198	0	VAL	Α	96	41.906	16.892	-3.665	1.00	16.47	A
5	ATOM	199	N	VAL	Α	97	43.157	15.033	-3.888	1.00	16.80	A
-	ATOM	200	CA	VAL		97	42.338	14.471	-4.949	1.00		A
	MOTA	201	СВ	VAL	Α	97	43.153	14.354	-6.255	1.00	18.43	A
	ATOM	202	CG1	VAL	Α	97	42.249	13.927	-7.404	1.00	19.69	A
	ATOM	203	CG2	VAL	Α	97	43.831	15.685	-6.569	1.00	17.84	A
10	ATOM	204	C	VAL		97	41.812	13.091	-4.583	1.00		A
10												
	ATOM	205	0	VAL	А	97	42.532	12.270	-4.014	1.00	1/.13	A
	ATOM	206	N	LEU	Α	98	40.545	12.845	-4.895	1.00	16.62	A
	ATOM	207	CA	LEU	Α	98	39.947	11.548	-4.624	1.00	17.04	A
	ATOM	208	СВ	LEU		98	38.424	11.633	-4.743	1.00		A
1.5												
15	ATOM	209	CG	LEU		98	37.635	10.342	-4.508	1.00		A
	ATOM	210	CD1	LEU	Α	98	37.990	9.762	-3.146	1.00	20.07	A
	ATOM	211	CD2	LEU	А	98	36.143	10.627	-4.588	1.00	17.93	A
		212	C	LEU		98	40.512	10.597	-5.677	1.00		A
	ATOM											
	MOTA	213	0	LEU	Α	98	40.527	10.920	-6.863	1.00		A
20	ATOM	214	N	ALA	Α	99	40.995	9.438	-5.246	1.00	17.13	A
	ATOM	215	CA	ALA	Α	99	41.570	8.466	-6.168	1.00	18.42	А
		216	СВ	ALA		99	43.090	8.524	-6.105	1.00		
	ATOM											A
	ATOM	217	С	ALA	Α	99	41.102	7.055	-5.848	1.00		A
	ATOM	218	0	ALA	Α	99	40.941	6.691	-4.679	1.00	22.52	A
25	ATOM	219	N	ARG	Α	100	40.878	6.261	-6.888	1.00	19.77	А
23				ARG				4.884		1.00		
	MOTA	220	CA				40.459		-6.693			A
	ATOM	221	СВ	ARG	Α	100	39.202	4.585	-7.518	1.00	24.22	A
	ATOM	222	CG	ARG	Α	100	38.608	3.205	-7.256	1.00	31.78	A
	ATOM	223	CD	ARG	Α	100	37.326	2.979	-8.048	1.00	36.24	А
30								3.818	-7.594			
30	ATOM	224	NE	ARG			36.213			1.00		A
	MOTA	225	CZ	ARG			35.566	3.662	-6.439	1.00		A
	ATOM	226	NH1	ARG	Α	100	35.912	2.696	-5.598	1.00	40.67	A
	ATOM	227	NH2	ARG	Α	100	34.559	4.468	-6.128	1.00	43.65	A
	ATOM	228	С	ARG			41.613	3.985	-7.129	1.00		A
2.5												
35	MOTA	229	0	ARG			42.078	4.065	-8.271	1.00		A
	ATOM	230	N	GLU	Α	101	42.102	3.157	-6.212	1.00	16.43	A
	ATOM	231	CA	GLU	Α	101	43.196	2.246	-6.533	1.00	16.11	A
	ATOM	232	СВ	GLU			43.774	1.637	-5.248	1.00		A
4.0	ATOM	233	CG	GLU			44.917	0.657	-5.488	1.00		A
40	ATOM	234	$^{\rm CD}$	GLU	Α	101	45.501	0.115	-4.200	1.00	18.20	A
	ATOM	235	OE1	GLU	Α	101	44.733	-0.081	-3.239	1.00	18.32	A
	ATOM	236	OE 2	GLU	Δ	101	46.725	-0.132	-4.150	1.00	17.14	A
	ATOM	237	C	GLU			42.625	1.152	-7.442	1.00		
												A
	ATOM	238	0	GLU			41.681	0.462	-7.069	1.00		A
45	MOTA	239	N	LEU	Α	102	43.198	1.002	-8.632	1.00	19.06	A
	ATOM	240	CA	LEU	Α	102	42.718	0.025	-9.607	1.00	20.71	A
	ATOM	241	СВ	LEU			43.569		-10.878	1.00		
												A
	MOTA	242	CG	LEU			43.531		-11.642	1.00		A
	ATOM	243	CD1	LEU	Α	102	44.577	1.414	-12.748	1.00	27.88	A
50	ATOM	244	CD2	LEU	А	102	42.140	1.647	-12.214	1.00	26.79	А
			C	LEU				-1.418	-9.125	1.00		
	ATOM	245					42.671					A
	ATOM	246	0	LEU			41.668	-2.103	-9.305	1.00		A
	MOTA	247	N	ALA	Α	103	43.753	-1.874	-8.507	1.00	19.38	A
	ATOM	248	CA	ALA			43.836	-3.249	-8.035	1.00		А
55	ATOM	249	CB	ALA			45.284	-3.571	-7.671	1.00		A
55												
	MOTA	250	С	ALA			42.919	-3.629	-6.872	1.00		A
	ATOM	251	0	ALA	Α	103	42.703	-4.815	-6.628	1.00	20.38	A
	ATOM	252	N	THR			42.361	-2.643	-6.175	1.00	18.12	А
	ATOM	253	CA	THR			41.517	-2.927	-5.018	1.00		A
	VI OIJ	200	υA	TIIL	17	T O 4	11. OT /	4.341	J. UIO	1. 00	11.1J	A

	MOTA	254	СВ	THR	Α	104	42.212	-2.484	-3.717	1.00 19.54	А
	MOTA	255		THR			42.456	-1.070	-3.773	1.00 19.26	A
	MOTA	256	CG2	THR			43.536	-3.219	-3.529	1.00 17.02	A
	MOTA	257	С	THR	Α	104	40.159	-2.247	-5.026	1.00 19.44	A
5	MOTA	258	0	THR	Α	104	39.259	-2.648	-4.285	1.00 18.70	A
	MOTA	259	N	SER	Α	105	40.034	-1.207	-5.847	1.00 19.65	A
	MOTA	260	CA	SER	Α	105	38.819	-0.400	-5.967	1.00 19.37	A
	MOTA	261	СВ	SER	Α	105	37.598	-1.304	-6.173	1.00 21.81	A
	MOTA	262	OG	SER	Α	105	36.431	-0.539	-6.412	1.00 23.01	A
10	MOTA	263	С	SER	Α	105	38.644	0.447	-4.701	1.00 18.99	A
	MOTA	264	0	SER	A	105	37.602	1.070	-4.488	1.00 18.66	A
	MOTA	265	N	ARG	Α	106	39.674	0.468	-3.861	1.00 16.84	А
	MOTA	266	CA	ARG	A	106	39.655	1.267	-2.634	1.00 16.21	A
	MOTA	267	СВ	ARG	Α	106	40.827	0.886	-1.723	1.00 16.41	A
15	MOTA	268	CG	ARG	Α	106	40.619	-0.367	-0.906	1.00 15.49	A
	MOTA	269	CD	ARG	Α	106	41.887	-0.755	-0.170	1.00 17.43	A
	MOTA	270	NE	ARG	Α	106	41.620	-1.792	0.824	1.00 20.47	A
	ATOM	271	CZ	ARG	Α	106	42.548	-2.568	1.371	1.00 20.24	A
	ATOM	272	NH1	ARG	Α	106	43.821	-2.433	1.017	1.00 17.80	А
20	ATOM	273	NH2	ARG	Α	106	42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG	Α	106	39.785	2.746	-2.981	1.00 17.37	A
	ATOM	275	0	ARG	Α	106	40.514	3.103	-3.902	1.00 17.75	A
	ATOM	276	N	GLU	Α	107	39.085	3.599	-2.240	1.00 16.06	А
	ATOM	277	CA	GLU	Α	107	39.156	5.039	-2.461	1.00 20.80	А
25	ATOM	278	СВ	GLU	Α	107	37.779	5.694	-2.337	1.00 22.93	A
	ATOM	279	CG	GLU	Α	107	36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	GLU	Α	107	35.431	5.975	-3.148	1.00 32.40	A
	ATOM	281	OE1	GLU	Α	107	35.262	6.939	-3.923	1.00 33.74	A
	ATOM	282	OE2	GLU	Α	107	34.608	5.654	-2.263	1.00 36.00	А
30	ATOM	283	С	GLU	Α	107	40.053	5.678	-1.410	1.00 18.93	А
	ATOM	284	0	GLU	Α	107	39.891	5.427	-0.220	1.00 19.21	А
	ATOM	285	N	TYR			40.988	6.507	-1.852	1.00 16.70	А
	ATOM	286	CA	TYR			41.883	7.209	-0.942	1.00 15.86	А
	ATOM	287	СВ	TYR			43.325	6.728	-1.104	1.00 15.30	А
35	ATOM	288	CG	TYR	Α	108	43.593	5.328	-0.612	1.00 16.33	A
	ATOM	289	CD1	TYR			43.765	5.066	0.746	1.00 16.36	A
	ATOM	290		TYR			44.046	3.769	1.201	1.00 18.48	А
	ATOM	291	CD2				43.701	4.268	-1.511	1.00 13.25	A
	ATOM	292		TYR			43.980	2.981	-1.075	1.00 17.28	A
40	ATOM	293	CZ	TYR			44.152	2.736	0.276	1.00 19.17	A
	ATOM	294	OH	TYR			44.440	1.461	0.688	1.00 19.38	A
	ATOM	295	C	TYR			41.850	8.687	-1.292	1.00 16.80	A
	ATOM	296	0	TYR			41.560	9.058	-2.431	1.00 15.22	A
	ATOM	297	N	ALA			42.132	9.528	-0.306	1.00 14.61	A
45	ATOM	298	CA	ALA			42.207	10.957	-0.539	1.00 14.30	A
	ATOM	299	СВ	ALA			41.671	11.726	0.661	1.00 14.78	A
	ATOM	300	C	ALA			43.713	11.136	-0.667	1.00 16.79	A
	ATOM	301	0	ALA			44.450	10.983	0.317	1.00 16.52	A
	ATOM	302	N	ILE			44.182	11.410	-1.881	1.00 14.80	A
50	ATOM	303	CA	ILE			45.609	11.574	-2.093	1.00 15.80	A
20	ATOM	304	СВ	ILE			46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305		ILE			47.550	11.098	-3.632	1.00 16.80	A
	ATOM	306		ILE			45.774	9.358	-3.284	1.00 17.76	A
	ATOM	307		ILE			46.308	8.513	-4.437	1.00 17.70	A
55	ATOM	308	CDI	ILE			46.004	13.045	-2.129	1.00 10.07	A
55	ATOM	309	0	ILE			45.534	13.813	-2.976	1.00 17.70	A
	ATOM	310	N	LYS			46.846	13.435	-2.970 -1.177	1.00 16.24	A
	ATOM	311	CA	LYS			47.326	14.808	-1.100	1.00 17.20	A
	ATOM	312	CB	LYS			47.700	15.176	0.344	1.00 17.20	A
	AIOM	J 14	CD	пто	М	T T T	11.700	TO.T/0	0.344	T.00 I/.41	A

	ATOM	313	CG	LYS A	A 111	48.350	16.547	0.464	1.00 20.71	А
	ATOM	314	CD		111	48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE		111	47.288	17.381	2.598	1.00 29.46	A
	ATOM	316	NZ		111	47.516	17.866	4.000	1.00 30.50	A
5	ATOM	317	C		111	48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	0		111	49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N		1112	48.509	15.798	-2.963	1.00 15.87	A
	ATOM	320	CA		1112	49.606	15.967	-3.907	1.00 17.28	A
	ATOM	321	CB		112	49.079	15.911	-5.358	1.00 17.20	A
10	ATOM	322	CG2	ILE A		50.235	15.998	-6.341	1.00 15.12	A
10	ATOM	323		ILE 2		48.293	14.609	-5.565	1.00 15.12	A
	ATOM	324		ILE A	112	47.580	14.511	-6.904	1.00 18.47 1.00 19.03	A
	ATOM	325	С			50.307	17.301	-3.663		A
1.5	ATOM	326	0		112	49.669	18.350	-3.635	1.00 19.15	A
15	ATOM	327	N		113	51.622	17.245	-3.472	1.00 20.22	A
	ATOM	328	CA	LEU A		52.416	18.442	-3.214	1.00 22.36	A
	ATOM	329	СВ		113	52.995	18.397	-1.794	1.00 22.13	A
	ATOM	330	CG		113	52.042	18.063	-0.646	1.00 22.46	A
	ATOM	331		LEU A		51.866	16.557	-0.553	1.00 23.81	A
20	ATOM	332		LEU A		52.603	18.595	0.660	1.00 23.68	А
	MOTA	333	С		113	53.560	18.547	-4.215	1.00 23.37	A
	ATOM	334	0		113	54.300	17.586	-4.424	1.00 23.11	A
	ATOM	335	N	GLU Z		53.706	19.714	-4.834	1.00 23.88	A
	ATOM	336	CA	GLU Z	114	54.771	19.920	-5.806	1.00 26.00	A
25	ATOM	337	СВ	GLU Z	114	54.435	21.111	-6.706	1.00 27.74	A
	MOTA	338	CG	GLU A	114	55.533	21.452	-7.696	1.00 35.07	A
	MOTA	339	CD	GLU Z	114	55.220	22.696	-8.497	1.00 39.24	A
	MOTA	340	OE1	GLU Z	114	54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU A	114	55.395	22.670	-9.736	1.00 44.05	A
30	ATOM	342	С	GLU A	114	56.087	20.163	-5.067	1.00 24.37	A
	ATOM	343	0	GLU Z	114	56.186	21.071	-4.238	1.00 24.43	A
	ATOM	344	N	LYS A	115	57.096	19.350	-5.360	1.00 24.10	A
	ATOM	345	CA	LYS A	115	58.376	19.493	-4.678	1.00 24.93	A
	ATOM	346	СВ		115	59.339	18.373	-5.103	1.00 23.72	A
35	ATOM	347	CG		115	59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD		115	60.064	15.944	-4.743	1.00 21.92	A
	ATOM	349	CE		115	59.691	15.400	-6.117	1.00 22.42	A
	ATOM	350	ΝZ		115	60.447	14.150	-6.448	1.00 19.71	A
	ATOM	351	С		115	59.031	20.858	-4.868	1.00 26.87	A
40	ATOM	352	0		115	59.492	21.469	-3.903	1.00 26.17	А
	ATOM	353	N		116	59.058	21.348	-6.102	1.00 28.73	А
	ATOM	354	CA		116	59.678	22.638	-6.380	1.00 29.66	A
	ATOM	355	СВ	ARG Z		59.533	22.980	-7.868	1.00 31.29	A
	ATOM	356	CG	ARG Z		60.047	24.361	-8.267	1.00 33.19	A
45	ATOM	357	CD	ARG Z		61.368	24.710	-7.590	1.00 35.13	A
	ATOM	358	NE	ARG Z		62.329	23.612	-7.618	1.00 36.42	A
	ATOM	359	CZ	ARG A		63.510	23.648	-7.009	1.00 36.18	A
	ATOM	360		ARG A		63.871	24.729	-6.332	1.00 36.12	A
	ATOM	361		ARG A		64.324	22.602	-7.067	1.00 35.77	A
50	ATOM	362	C	ARG Z		59.097	23.761	-5.519	1.00 29.70	A
20	ATOM	363	0	ARG A		59.843	24.515	-4.889	1.00 29.16	A
	ATOM	364	N	HIS A		57.773	23.862	-5.472	1.00 27.22	A
	ATOM	365	CA	HIS Z		57.126	24.903	-4.681	1.00 27.22	A
	ATOM	366	CB	HIS A		55.606	24.903	-4.848	1.00 28.33	A
55	ATOM	367	СБ	HIS Z		54.881	26.005	-4.258	1.00 28.41	A
55	ATOM	368		HIS A		55.309	27.249	-3.935	1.00 31.02	A A
	ATOM ATOM	369		HIS A		53.536	25.974	-3.935 -3.961	1.00 33.19	A A
		369 370								
	ATOM			HIS A		53.165	27.148	-3.480	1.00 34.58	A
	MOTA	371	ΝĽΖ	HIS A	-7 TT \	54.222	27.940	-3.455	1.00 35.18	A

	ATOM	372	С	HIS A	117	57.477	24.780	-3.202	1.00 26.22	A
	ATOM	373	0	HIS A	117	57.737	25.776	-2.534	1.00 25.67	A
	ATOM	374	N	ILE A		57.469	23.554	-2.689	1.00 24.94	A
	ATOM	375	CA	ILE A	118	57.792	23.315	-1.285	1.00 23.94	A
5	ATOM	376	СВ	ILE A	118	57.711	21.812	-0.952	1.00 23.50	A
	ATOM	377		ILE A		58.374	21.533	0.389	1.00 23.76	A
	ATOM	378	CG1	ILE A	118	56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379	CD1	ILE A	118	56.066	19.858	-0.834	1.00 28.06	A
	ATOM	380	С	ILE A	118	59.195	23.821	-0.958	1.00 23.78	A
10	ATOM	381	0	ILE A		59.402	24.495	0.048	1.00 23.49	А
10										
	ATOM	382	N	ILE A		60.153	23.489	-1.815	1.00 23.46	A
	ATOM	383	CA	ILE A	119	61.534	23.913	-1.619	1.00 25.13	A
	ATOM	384	СВ	ILE A	119	62.467	23.250	-2.664	1.00 24.25	A
	ATOM	385	CG2	ILE A		63.858	23.890	-2.617	1.00 22.47	А
1.5										
15	ATOM	386		ILE A		62.540	21.738	-2.395	1.00 25.05	A
	ATOM	387	CD1	ILE A	119	63.327	20.945	-3.439	1.00 24.62	A
	ATOM	388	С	ILE A	119	61.667	25.435	-1.705	1.00 25.96	A
	ATOM	389	0	ILE A		62.330	26.051	-0.872	1.00 24.78	А
									1.00 27.67	
	ATOM	390	N	LYS A		61.028	26.039	-2.704		A
20	ATOM	391	CA	LYS A	120	61.100	27.489	-2.879	1.00 30.29	A
	ATOM	392	CB	LYS A	120	60.242	27.940	-4.060	1.00 32.34	A
	ATOM	393	CG	LYS A		60.674	27.407	-5.409	1.00 39.30	А
	ATOM	394	CD	LYS A		59.765	27.950	-6.512	1.00 45.19	A
	ATOM	395	CE	LYS A	120	58.294	27.636	-6.218	1.00 46.48	A
25	ATOM	396	NZ	LYS A	120	57.363	28.155	-7.252	1.00 46.49	A
	ATOM	397	С	LYS A	120	60.647	28.247	-1.638	1.00 30.89	А
	ATOM	398	0	LYS A		61.303	29.198	-1.217	1.00 32.48	A
	ATOM	399	N	GLU A	121	59.527	27.825	-1.055	1.00 29.82	A
	ATOM	400	CA	GLU A	121	58.986	28.488	0.128	1.00 30.33	A
30	ATOM	401	СВ	GLU A	121	57.455	28.416	0.117	1.00 33.04	A
	ATOM	402	CG	GLU A		56.794	29.021	-1.120	1.00 36.45	A
	ATOM	403	CD	GLU A		57.221	30.456	-1.373	1.00 39.88	A
	ATOM	404	OE1	GLU A	121	57.200	31.264	-0.420	1.00 40.53	A
	ATOM	405	OE2	GLU A	121	57.573	30.778	-2.529	1.00 43.24	A
35	ATOM	406	C	GLU A		59.511	27.930	1.451	1.00 30.37	A
33										
	ATOM	407	0	GLU A		58.946	28.204	2.513	1.00 31.24	A
	ATOM	408	N	ASN A	122	60.588	27.151	1.390	1.00 29.03	A
	ATOM	409	CA	ASN A	122	61.183	26.573	2.594	1.00 28.46	A
	ATOM	410	СВ	ASN A		61.836	27.673	3.436	1.00 31.28	A
40										
40	ATOM	411	CG	ASN A		62.945	28.395	2.698	1.00 34.12	A
	ATOM	412	OD1	ASN A	122	62.697	29.143	1.754	1.00 35.57	A
	ATOM	413	ND2	ASN A	122	64.181	28.169	3.127	1.00 35.73	A
	ATOM	414	С	ASN A	122	60.157	25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN A		60.085	26.055	4.663	1.00 27.23	A
4.5										
45	ATOM	416	N	LYS A		59.375	24.955	2.842	1.00 23.99	A
	ATOM	417	CA	LYS A	123	58.358	24.210	3.574	1.00 22.43	A
	ATOM	418	СВ	LYS A	123	57.031	24.248	2.810	1.00 21.97	A
	ATOM	419	CG	LYS A		56.475	25.645	2.599	1.00 25.68	A
	ATOM	420	CD	LYS A		56.253	26.354	3.927	1.00 27.54	A
50	ATOM	421	CE	LYS A	123	55.822	27.796	3.716	1.00 31.30	A
	ATOM	422	NZ	LYS A	123	55.756	28.540	5.004	1.00 33.21	A
	ATOM	423	С	LYS A		58.748	22.759	3.821	1.00 22.20	А
	ATOM	424	0	LYS A		57.924	21.960	4.264	1.00 22.50	A
	ATOM	425	N	VAL A	124	59.997	22.412	3.535	1.00 20.59	A
55	ATOM	426	CA	VAL A	124	60.439	21.039	3.730	1.00 20.25	A
	ATOM	427	СВ	VAL A	124	61.922	20.850	3.328	1.00 19.43	А
		428							1.00 18.69	
	ATOM			VAL A		62.346	19.407	3.573		A
	ATOM	429		VAL A		62.104	21.195	1.853	1.00 18.21	A
	ATOM	430	С	VAL A	124	60.236	20.561	5.163	1.00 19.53	A

	ATOM	431	0	VAL	Α	124	59.841	19.418	5.385	1.00	20.02	A
		432		PRO	70	105						
	ATOM		Ν				60.513	21.422	6.159		20.01	A
	ATOM	433	$^{\rm CD}$	PRO	Α	125	61.178	22.738	6.118	1.00	18.69	A
	ATOM	434	CA	PRO	Δ	125	60.318	20.979	7.544	1 00	19.88	А
_												
5	MOTA	435	СВ	PRO			60.793	22.180	8.363		19.95	A
	ATOM	436	CG	PRO	Α	125	61.839	22.805	7.479	1.00	18.85	A
	ATOM	437	С	PRO	Ζ	125	58.848	20.642	7.824	1 00	19.76	А
	ATOM	438	0	PRO	Α	125	58.544	19.700	8.550	1.00	16.99	A
	MOTA	439	N	TYR	Α	126	57.947	21.418	7.235	1.00	18.98	A
10	ATOM	440	CA	TYR			56.516	21.220	7.435		21.97	А
10												
	MOTA	441	CB	TYR	Α	126	55.752	22.448	6.933		25.17	A
	ATOM	442	CG	TYR	Α	126	56.040	23.690	7.748	1.00	30.98	A
		443		TYR			55.438	23.886	8.991		33.95	
	MOTA											A
	MOTA	444	CE1	TYR	Α	126	55.721	25.015	9.763	1.00	36.60	A
15	ATOM	445	CD2	TYR	Α	126	56.938	24.657	7.292	1.00	35.43	A
	ATOM	446		TYR			57.231	25.792	8.058		37.20	A
	ATOM	447	CZ	TYR	Α	126	56.618	25.962	9.291	1.00	37.40	A
	ATOM	448	OH	TYR	Δ	126	56.903	27.073	10.052	1 00	40.85	А
	ATOM	449	С	TYR			55.990	19.956	6.762		21.35	A
20	ATOM	450	0	TYR	Α	126	55.265	19.175	7.383	1.00	20.49	A
	ATOM	451	N	VAL	Δ	127	56.354	19.746	5.501	1 00	18.16	А
	ATOM	452	CA	VAL			55.892	18.562	4.790		17.58	A
	ATOM	453	CB	VAL	Α	127	56.308	18.596	3.308	1.00	17.45	A
	ATOM	454	CG1	VAL			55.786	17.350	2.600	1 00	17.97	А
2.5												
25	ATOM	455	CG2	VAL			55.751	19.850	2.641		14.90	A
	ATOM	456	С	VAL	Α	127	56.459	17.306	5.448	1.00	18.39	A
	ATOM	457	0	VAL	7	127	55.769	16.298	5.583	1 00	18.14	А
	ATOM	458	N	THR	А	128	57.716	17.381	5.869	1.00	17.50	A
	ATOM	459	CA	THR	Α	128	58.375	16.260	6.530	1.00	18.54	A
30	ATOM	460	СВ	THR			59.861	16.586	6.805		18.01	A
30												
	MOTA	461	OG1	THR	Α	128	60.537	16.804	5.559	1.00	21.14	A
	ATOM	462	CG2	THR	Α	128	60.536	15.446	7.545	1.00	17.95	A
	ATOM	463	С	THR			57.676	15.941	7.856		19.49	A
	ATOM	464	0	THR	Α	128	57.438	14.776	8.179	1.00	18.76	A
35	ATOM	465	N	ARG	Α	129	57.345	16.981	8.619	1.00	19.60	A
	ATOM	466		ARG			56.673	16.804	9.904		20.12	A
			CA									
	ATOM	467	CB	ARG	Α	129	56.534	18.144	10.621	1.00	21.33	A
	ATOM	468	CG	ARG	Α	129	55.948	18.029	12.023	1.00	28.02	A
				ARG							31.25	
	MOTA	469	CD				55.721	19.404	12.597			A
40	ATOM	470	NE	ARG	Α	129	56.940	20.205	12.560	1.00	37.78	A
	ATOM	471	CZ	ARG	Α	129	56.962	21.524	12.391	1.00	40.10	A
	ATOM	472		ARG			55.828	22.197	12.239		40.03	
												A
	MOTA	473	NH2	ARG	Α	129	58.119	22.170	12.374	1.00	44.58	A
	MOTA	474	С	ARG	Α	129	55.288	16.186	9.729	1.00	20.08	A
45	ATOM	475	0	ARG			54.891	15.305	10.496		20.40	А
45												
	ATOM	476	N	GLU	Α	130	54.553	16.654	8.724	1.00	18.79	A
	MOTA	477	CA	GLU	Α	130	53.222	16.125	8.454	1.00	20.10	A
	ATOM	478	СВ	GLU			52.638	16.749	7.183		19.92	A
	MOTA	479	CG	GLU	Α	130	51.350	16.087	6.708	1.00	27.85	A
50	MOTA	480	CD	GLU	Α	130	50.581	16.933	5.707	1.00	29.72	A
				GLU								
	ATOM	481					51.216	17.528	4.814		33.46	A
	MOTA	482	OE2	GLU	Α	130	49.339	16.996	5.807	1.00	30.74	A
	ATOM	483	С	GLU			53.301	14.615	8.295		19.81	А
	ATOM	484	0	GLU			52.553	13.875	8.935		18.37	A
55	MOTA	485	N	ARG	Α	131	54.219	14.162	7.447	1.00	20.41	A
	ATOM	486	CA	ARG			54.397	12.735	7.202		22.45	А
	ATOM	487	СВ	ARG			55.442	12.511	6.098		25.16	А
	MOTA	488	CG	ARG	Α	131	55.742	11.043	5.840	1.00	28.75	A
	ATOM	489	CD	ARG			56.736	10.837	4.708		33.75	А
	111 011	100	OD.	21210	- 1		50.750	10.007	1.700	00	20.70	11

	ATOM	490	NE	ARG	Α	131	57.020	9.415	4.520	1.00	40.07	A
	ATOM	491	CZ	ARG	Ζ	131	57.756	8.915	3.532	1 00	43.07	А
	ATOM	492		ARG			58.293	9.721	2.625		44.91	A
	ATOM	493	NH2	ARG	Α	131	57.955	7.606	3.449	1.00	44.45	A
5	ATOM	494	С	ARG	Δ	131	54.820	11.982	8.466	1 00	23.24	А
5												
	ATOM	495	0	ARG			54.241	10.948	8.804		23.86	A
	ATOM	496	N	ASP	Α	132	55.831	12.497	9.160	1.00	21.99	A
	ATOM	497	CA	ASP	Α	132	56.318	11.850	10.370	1.00	22.04	A
	ATOM	498	СВ	ASP			57.570	12.564	10.888		23.72	A
10												
10	ATOM	499	CG	ASP			58.750	12.442	9.932		27.77	A
	ATOM	500	od1	ASP	Α	132	58.681	11.620	8.989	1.00	27.34	A
	ATOM	501	OD2	ASP	Α	132	59.753	13.163	10.128	1.00	28.70	А
	ATOM	502	C	ASP			55.258	11.772	11.474		21.69	A
	ATOM	503	0	ASP	А	132	55.077	10.723	12.092	1.00	22.75	A
15	ATOM	504	N	VAL	Α	133	54.551	12.868	11.725	1.00	19.54	A
	ATOM	505	CA	VAL	Α	133	53.525	12.843	12.759	1.00	18.52	А
		506	СВ	VAL			52.908	14.244	12.990		19.26	A
	ATOM											
	ATOM	507	CG1	VAL	Α	133	51.708	14.135	13.918	1.00	18.79	A
	ATOM	508	CG2	VAL	Α	133	53.953	15.180	13.604	1.00	18.80	A
20	ATOM	509	С	VAL	Δ	133	52.419	11.854	12.398	1.00	19.46	А
20												
	ATOM	510	0	VAL			52.073	10.991	13.200		19.94	A
	ATOM	511	N	MET	Α	134	51.878	11.957	11.187	1.00	19.15	A
	ATOM	512	CA	MET	Α	134	50.807	11.052	10.792	1.00	21.25	A
	ATOM	513	СВ	MET			50.309	11.381	9.383		17.34	А
25												
25	ATOM	514	CG	MET			49.615	12.730	9.302		20.00	A
	ATOM	515	SD	MET	Α	134	48.643	12.952	7.798	1.00	24.21	A
	ATOM	516	CE	MET	Α	134	47.033	12.434	8.400	1.00	23.20	A
	ATOM	517	С	MET			51.203	9.582	10.881		22.43	A
	ATOM	518	0	MET			50.384	8.741	11.249		23.82	A
30	ATOM	519	N	SER	Α	135	52.454	9.273	10.556	1.00	23.09	A
	ATOM	520	CA	SER	Α	135	52.939	7.895	10.615	1.00	26.13	А
		521		SER			54.356	7.798	10.039		26.17	A
	ATOM		СВ									
	ATOM	522	OG	SER	Α	135	54.383	8.177	8.673	1.00	31.91	A
	ATOM	523	С	SER	Α	135	52.957	7.358	12.045	1.00	26.58	A
35	ATOM	524	0	SER	Δ	135	52.926	6.148	12.261		26.42	A
55		525					53.014	8.261			25.65	
	ATOM		N	ARG					13.018			A
	ATOM	526	CA	ARG	Α	136	53.056	7.870	14.425	1.00	27.47	A
	ATOM	527	СВ	ARG	Α	136	53.823	8.914	15.238	1.00	27.97	A
	ATOM	528	CG	ARG	Δ	136	55.283	9.082	14.857	1.00	32.00	А
40		529		ARG							33.03	
40	ATOM		CD				55.904	10.218	15.664			A
	ATOM	530	NE	ARG	Α	136	55.602	10.073	17.084	1.00	36.11	A
	ATOM	531	CZ	ARG	Α	136	55.867	10.990	18.007	1.00	39.74	A
	ATOM	532	NH1	ARG	Δ	136	56.449	12.132	17.661	1.00	40.55	A
	ATOM	533		ARG			55.540	10.769	19.276		36.72	
												A
45	ATOM	534	С	ARG	Α	136	51.667	7.709	15.036	1.00	26.38	A
	ATOM	535	0	ARG	Α	136	51.516	7.121	16.106	1.00	27.06	A
	ATOM	536	N	LEU	Δ	137	50.655	8.235	14.360		24.77	A
	ATOM	537	CA	LEU			49.294	8.162	14.870		24.70	A
	ATOM	538	СВ	LEU	Α	137	48.483	9.363	14.371	1.00	24.52	A
50	ATOM	539	CG	LEU	Α	137	49.050	10.760	14.662	1.00	26.67	A
	ATOM	540	CD1	LEU	Δ	137	48.075	11.813	14.141		27.25	А
	ATOM	541		LEU			49.279	10.945	16.155		27.09	А
	ATOM	542	С	LEU	Α	137	48.592	6.868	14.473	1.00	25.20	A
	ATOM	543	0	LEU	Α	137	48.619	6.469	13.309	1.00	25.99	A
55	ATOM	544	N	ASP			47.971	6.218	15.451		21.89	А
55												
	ATOM	545	CA	ASP			47.239	4.977	15.219		21.35	A
	ATOM	546	СВ	ASP	Α	138	48.124	3.761	15.523	1.00	22.14	А
	ATOM	547	CG	ASP	Α	138	47.432	2.448	15.201	1.00	24.90	A
	ATOM	548		ASP			46.631	2.423	14.241		24.78	A
	111 011	0.10	\circ_D $_{\perp}$	110 L	11	100	10.001	2.425	_ 1 • 2 7 1	1.00	21.70	А

	ATOM	549	OD2	ASP A	138	47.691	1.443	15.897	1.00 25.39	А
	ATOM	550	C	ASP A		46.031	4.991	16.138	1.00 20.47	
	ATOM	551	0	ASP A		45.967	4.248	17.118	1.00 19.06	
	ATOM	552	N	HIS A		45.075	5.852	15.810	1.00 18.27	
5	ATOM	553	CA	HIS A		43.869	6.016	16.606	1.00 18.21	
3										
	ATOM	554	CB	HIS A		44.096	7.157	17.612	1.00 15.84	A
	ATOM	555	CG	HIS A		42.985	7.332	18.600	1.00 15.24	
	ATOM	556		HIS A		42.884	6.964	19.900	1.00 13.97	
10	ATOM	557		HIS A		41.791	7.943	18.280	1.00 14.74	
10	ATOM	558		HIS A		41.002	7.944	19.341	1.00 14.19	A
	ATOM	559		HIS A		41.641	7.356	20.336	1.00 14.15	
	ATOM	560	С	HIS A		42.715	6.330	15.654	1.00 18.50	
	ATOM	561	0	HIS A		42.879	7.080	14.693	1.00 20.80	
	ATOM	562	N	PRO A	140	41.527	5.767	15.913	1.00 18.32	A
15	ATOM	563	CD	PRO A	140	41.143	4.984	17.100	1.00 16.71	A
	ATOM	564	CA	PRO A	140	40.367	6.001	15.048	1.00 17.43	A
	ATOM	565	СВ	PRO A	140	39.273	5.157	15.704	1.00 16.64	A
	ATOM	566	CG	PRO A	140	39.643	5.204	17.152	1.00 18.43	А
	ATOM	567	С	PRO A	140	39.914	7.441	14.803	1.00 18.77	А
20	ATOM	568	0	PRO A	140	39.207	7.695	13.831	1.00 19.88	
	ATOM	569	N	PHE A		40.301	8.381	15.664	1.00 17.14	A
	ATOM	570	CA	PHE A		39.874	9.767	15.477	1.00 16.42	
	ATOM	571	СВ	PHE A		39.568	10.422	16.836	1.00 14.60	A
	ATOM	572	CG	PHE A		38.386	9.817	17.556	1.00 15.26	
25	ATOM	573		PHE A		37.335	9.234	16.842	1.00 14.78	
23	ATOM	574		PHE A		38.297	9.880	18.942	1.00 13.70	
	ATOM	575		PHE A		36.215	8.727	17.502	1.00 16.94	
	ATOM	576		PHE A		37.178	9.375	19.615	1.00 15.75	
30	ATOM	577	CZ	PHE A		36.135	8.799	18.893	1.00 16.89 1.00 16.15	
30	ATOM	578 570	C	PHE A		40.857	10.641	14.694		
	ATOM	579	0	PHE A		40.799	11.871	14.761	1.00 17.35	
	ATOM	580	N	PHE A		41.748	10.011	13.941	1.00 15.88	A
	ATOM	581	CA	PHE A		42.727	10.756	13.154	1.00 17.89	
	ATOM	582	СВ	PHE A		44.115	10.645	13.793	1.00 17.57	
35	ATOM	583	CG	PHE A		44.240	11.371	15.103	1.00 18.74	
	ATOM	584		PHE A		44.559	12.726	15.135	1.00 17.77	
	ATOM	585		PHE A		43.997	10.711	16.304	1.00 18.74	
	MOTA	586	CE1	PHE A	142	44.632	13.417	16.347	1.00 15.77	A
	ATOM	587	CE2	PHE A		44.065	11.393	17.522	1.00 17.56	A
40	ATOM	588	CZ	PHE A	142	44.383	12.747	17.542	1.00 17.14	A
	ATOM	589	С	PHE A	142	42.793	10.231	11.729	1.00 19.12	A
	ATOM	590	0	PHE A	142	42.659	9.030	11.504	1.00 20.01	A
	ATOM	591	N	VAL A	143	42.978	11.135	10.769	1.00 18.72	A
	ATOM	592	CA	VAL A	143	43.102	10.735	9.371	1.00 18.52	А
45	ATOM	593	СВ	VAL A		43.294	11.961	8.440	1.00 20.66	
	ATOM	594	CG1	VAL A	143	43.843	11.521	7.080	1.00 21.29	А
	ATOM	595		VAL A		41.958	12.673	8.252	1.00 22.97	А
	ATOM	596	С	VAL A		44.342	9.865	9.330	1.00 18.68	A
	ATOM	597	0	VAL A		45.355	10.199	9.943	1.00 18.42	A
50	ATOM	598	N	LYS A		44.259	8.745	8.623	1.00 18.30	A
20	ATOM	599	CA	LYS A		45.384	7.824	8.535	1.00 18.78	A
	ATOM	600	CB	LYS A		44.889	6.373	8.608	1.00 22.27	A
	ATOM	601	CG	LYS A		46.017	5.340	8.557	1.00 22.27	
		602	CD	LYS A		45.491	3.912	8.674	1.00 29.72	A
55	ATOM									A
55	ATOM	603	CE	LYS A		46.631	2.896	8.577	1.00 37.67	A
	ATOM	604	ΝZ	LYS A		46.138	1.484	8.629	1.00 39.02	A
	ATOM	605	C	LYS A		46.192	8.002	7.261	1.00 18.53	A
	ATOM	606	0	LYS A		45.643	8.314	6.200	1.00 18.18	A
	ATOM	607	N	LEU A	145	47.502	7.816	7.385	1.00 16.79	A

	ATOM	608	CA	LEU	Α	145	48.411	7.900	6.251	1.00	17.45	A
	ATOM	609	СВ	LEU	А	145	49.686	8.653	6.641	1.00	18.82	A
	ATOM	610	CG	LEU	Α	145	50.734	8.902	5.549	1.00	20.23	A
	ATOM	611		LEU			51.836	9.799	6.093		18.83	A
5	ATOM	612	CD2	LEU	Α	145	51.317	7.581	5.069	1.00	19.79	A
	ATOM	613	С	LEU	7\	1/15	48.739	6.450	5.907	1 00	19.19	А
	ATOM	614	0	LEU	Α	145	49.451	5.772	6.659	1.00	17.36	A
	ATOM	615	N	TYR	Α	146	48.215	5.972	4.782	1.00	17.28	A
									4.358		17.57	
	ATOM	616	CA	TYR			48.444	4.593				A
10	ATOM	617	СВ	TYR	Α	146	47.288	4.098	3.486	1.00	17.74	A
	ATOM	618	CG	TYR	Δ	146	45.981	3.926	4.214	1 00	17.50	А
	ATOM	619	CDI	TYR	А	146	45.099	4.995	4.377	1.00	16.50	A
	ATOM	620	CE1	TYR	Α	146	43.881	4.827	5.039	1.00	17.10	A
	ATOM	621		TYR			45.620	2.686	4.735		18.28	A
15	MOTA	622	CE2	TYR	Α	146	44.411	2.506	5.399	1.00	19.84	A
	ATOM	623	CZ	TYR	Α	146	43.547	3.576	5.544	1.00	17.53	A
	ATOM	624	OH	TYR	А	146	42.342	3.376	6.169		20.67	A
	ATOM	625	С	TYR	Α	146	49.735	4.376	3.582	1.00	18.72	A
	ATOM	626	0	TYR	7\	116	50.382	3.338	3.715	1 00	19.51	А
20												
20	ATOM	627	N	PHE	Α	147	50.110	5.350	2.765	1.00	18.09	A
	ATOM	628	CA	PHE	Α	147	51.307	5.203	1.952	1.00	17.20	A
	ATOM	629	СВ	PHE			51.007	4.258	0.783		16.77	А
	ATOM	630	CG	PHE	Α	147	49.835	4.699	-0.070	1.00	17.75	A
	ATOM	631	CD1	PHE	Δ	147	49.967	5.752	-0.975	1 00	16.58	А
2.5												
25	ATOM	632	CD2	PHE	А	14/	48.595	4.075	0.053	1.00	18.07	A
	ATOM	633	CE1	PHE	Α	147	48.886	6.178	-1.742	1.00	19.62	A
	ATOM	634		PHE			47.503	4.492	-0.710		18.56	А
	ATOM	635	CZ	PHE	Α	147	47.647	5.546	-1.610	1.00	19.27	A
	ATOM	636	С	PHE	Α	147	51.768	6.533	1.395	1.00	17.13	A
20												
30	ATOM	637	0	PHE			51.045	7.528	1.452		14.43	A
	MOTA	638	N	THR	Α	148	52.981	6.534	0.854	1.00	17.12	A
	ATOM	639	CA	THR	Δ	148	53.541	7.718	0.232	1 00	17.96	А
	ATOM	640	СВ	THR	А	148	54.449	8.531	1.197	1.00	21.51	A
	ATOM	641	OG1	THR	Α	148	55.605	7.760	1.537	1.00	18.83	A
35	ATOM	642		THR			53.700	8.897	2.472		19.60	А
33												
	MOTA	643	С	THR	Α	148	54.386	7.262	-0.946	1.00	20.31	A
	ATOM	644	0	THR	Ά	148	54.860	6.124	-0.991	1.00	18.94	A
	ATOM	645	N	PHE			54.543	8.149	-1.916		19.16	A
	ATOM	646	CA	PHE	Α	149	55.368	7.877	-3.073	1.00	18.01	A
40	ATOM	647	СВ	PHE	Δ	149	54.748	6.801	-3.989	1 00	17.23	А
10												
	ATOM	648	CG	PHE	А	149	53.389	7.144	-4.544	1.00	16.88	A
	ATOM	649	CD1	PHE	Α	149	53.262	7.888	-5.712	1.00	18.58	A
	ATOM	650		PHE			52.235	6.668	-3.927		17.31	А
	ATOM	651	CET	PHE	А	149	52.007	8.149	-6.267	1.00	19.26	A
45	ATOM	652	CE2	PHE	А	149	50.972	6.923	-4.470	1.00	19.17	A
				PHE			50.858	7.663	-5.642		19.60	
	ATOM	653	CZ									А
	ATOM	654	С	PHE	Α	149	55.542	9.205	-3.774	1.00	20.85	A
	ATOM	655	0	PHE	Δ	149	54.934	10.200	-3.376	1 00	19.76	A
	ATOM	656	N	GLN	А	150	56.398	9.241	-4.782		19.79	A
50	ATOM	657	CA	GLN	Α	150	56.636	10.481	-5.497	1.00	24.03	A
	ATOM	658	СВ	GLN	7\	150	57.659	11.347	-4.739		24.45	А
	ATOM	659	CG	GLN	Α	150	58.986	10.645	-4.414	1.00	26.28	A
	ATOM	660	CD	GLN	Α	150	59.988	11.558	-3.692	1.00	29.02	A
											27.05	
	ATOM	661		GLN			60.693	12.353	-4.321			A
55	ATOM	662	NE2	GLN	Α	150	60.042	11.449	-2.365	1.00	26.47	A
	ATOM	663	С	GLN	Ά	150	57.160	10.203	-6.885	1.00	23.88	А
	ATOM	664	0	GLN			57.673	9.118	-7.158		24.79	A
	ATOM	665	N	ASP	Α	151	56.987	11.171	-7.774	1.00	25.88	A
	ATOM	666	CA	ASP			57.527	11.047	-9.117		26.49	А
	14 T OLI	000	UA.	ANE	17	T O T	51.521	TT.01/	J • 11 1	1.00	20.70	A

	ATOM	667	СВ	ASP	Α	151	56.437	11.126	-10.199	1.00	24.54	A
	ATOM	668	CG	ASP	7	151	55.544	12 336	-10.064	1 00	24.95	А
	ATOM	669		ASP			56.005	13.379	-9.561		22.44	A
	ATOM	670	OD2	ASP	Α	151	54.369	12.242	-10.490	1.00	25.72	A
5	ATOM	671	С	ASP	ΖΔ.	151	58.515	12.203	-9.220	1 00	28.63	A
5								12.780			27.83	
	ATOM	672	0	ASP			58.890		-8.194			A
	ATOM	673	N	ASP	Α	152	58.934	12.560	-10.426	1.00	29.21	A
	ATOM	674	CA	ASP	Α	152	59.907	13.636	-10.562	1.00	31.88	A
	ATOM	675	СВ	ASP			60.325		-12.026		33.94	А
10												
10	ATOM	676	CG	ASP	А	152	61.033		-12.557		38.88	A
	ATOM	677	od1	ASP	Α	152	61.817	11.959	-11.791	1.00	39.67	A
	ATOM	678	OD2	ASP	Α	152	60.817	12.211	-13.738	1.00	41.57	А
	ATOM	679	C	ASP			59.487		-10.013		30.90	A
	ATOM	680	0	ASP			60.316	15.735	-9.482		31.69	A
15	ATOM	681	N	GLU	Α	153	58.207	15.322	-10.107	1.00	29.44	A
	ATOM	682	CA	GLU	Ά	153	57.767	16.632	-9.646	1.00	28.69	A
		683		GLU			56.984		-10.766		32.90	A
	ATOM		СВ									
	ATOM	684	CG	GLU	Α	153	57.451	16.987	-12.183	1.00	40.57	A
	ATOM	685	CD	GLU	Α	153	56.920	15.643	-12.675	1.00	45.78	A
20	ATOM	686	OE 1	GLU	Δ	153	55.682	15.482	-12.760	1.00	48.91	A
20									-12.979			
	ATOM	687		GLU			57.736				48.95	A
	ATOM	688	С	GLU	Α	153	56.929	16.683	-8.372		26.43	A
	ATOM	689	0	GLU	Α	153	56.947	17.688	-7.660	1.00	25.08	А
	ATOM	690	N	LYS			56.205	15.610	-8.069		22.39	А
25												
25	ATOM	691	CA	LYS			55.318	15.631	-6.912		21.43	A
	ATOM	692	СВ	LYS	Α	154	53.861	15.628	-7.398	1.00	20.33	A
	ATOM	693	CG	LYS	Α	154	53.505	16.716	-8.403	1.00	21.92	А
	ATOM	694	CD	LYS			52.211	16.375	-9.146		19.70	A
	ATOM	695	CE	LYS	Α	154	51.775	17.503	-10.077	1.00	20.04	A
30	ATOM	696	NZ	LYS	Α	154	50.631	17.094	-10.951	1.00	19.97	A
	ATOM	697	С	LYS	Δ	154	55.458	14.522	-5.881	1.00	20.43	A
		698		LYS			55.949	13.426	-6.173		21.13	
	ATOM		0									A
	ATOM	699	Ν	LEU	Α	155	54.985	14.832	-4.676	1.00	19.69	A
	ATOM	700	CA	LEU	Α	155	54.950	13.900	-3.553	1.00	19.10	A
35	ATOM	701	СВ	LEU	Δ	155	55.362	14.588	-2.252	1 00	19.65	A
55		702	CG					15.234			21.20	
	ATOM			LEU			56.740		-2.129			A
	ATOM	703	CD1	LEU	Α	155	56.848	15.918	-0.770	1.00	23.42	A
	ATOM	704	CD2	LEU	Α	155	57.816	14.174	-2.277	1.00	23.08	A
	ATOM	705	С	LEU	Δ	155	53.478	13.507	-3.427	1 00	18.87	А
40		706		LEU								
40	ATOM		0				52.600	14.348	-3.620		18.61	А
	ATOM	707	Ν	TYR	Α	156	53.209	12.249	-3.091	1.00	15.02	A
	ATOM	708	CA	TYR	Α	156	51.834	11.783	-2.934	1.00	16.29	A
	ATOM	709	СВ	TYR			51.470	10.769	-4.029		14.20	A
	ATOM	710	CG	TYR			51.603	11.273	-5.449		17.29	A
45	ATOM	711	CD1	TYR	Α	156	52.857	11.429	-6.045	1.00	16.46	A
	ATOM	712	CE1	TYR	Α	156	52.978	11.884	-7.360	1.00	18.68	A
	ATOM	713		TYR			50.474	11.588	-6.202		16.43	А
	ATOM	714	CEZ	TYR			50.583	12.048	-7.512		16.31	A
	ATOM	715	CZ	TYR	Α	156	51.835	12.192	-8.083	1.00	18.17	A
50	ATOM	716	OH	TYR	Α	156	51.941	12.651	-9.371	1.00	17.47	A
	ATOM	717	С	TYR			51.657	11.108	-1.572		16.32	А
	ATOM	718	0	TYR			52.412	10.197	-1.235		16.27	A
	ATOM	719	N	PHE	Α	157	50.678	11.568	-0.792	1.00	15.47	A
	ATOM	720	CA	PHE	Α	157	50.385	10.966	0.508		16.66	А
55	ATOM	721	СВ	PHE			50.324	12.014	1.629		16.91	A
55												
	ATOM	722	CG	PHE			51.631	12.708	1.907		18.96	A
	ATOM	723	CD1	PHE	Α	157	52.821	12.261	1.340	1.00	20.31	A
	ATOM	724	CD2	PHE	Α	157	51.664	13.829	2.732	1.00	21.12	A
		725		PHE				12.926	1.585		22.08	
	ATOM	120	CHI	E 1115	ч	T 0 1	54.025	14.940	1.000	1.00	22.00	A

	ATOM	726	CE2	PHE A	157	52.	.865	14.500	2.982	1.00	22.18	A
	ATOM	727	CZ	PHE A		5.4	.045	14.045	2.405	1 00	21.27	А
	MOTA	728	С	PHE A		49.	.016	10.308	0.404		16.52	A
	ATOM	729	0	PHE A	157	48.	.029	10.979	0.110	1.00	17.32	A
5	ATOM	730	N	GLY A	158	4.8	.953	9.002	0.644	1.00	15.97	A
-	ATOM	731	CA	GLY A			.684	8.299	0.572		16.13	A
	MOTA	732	С	GLY A		4 /	.000	8.383	1.920		14.94	A
	ATOM	733	0	GLY A	158	47.	.445	7.756	2.879	1.00	16.28	A
	ATOM	734	N	LEU A	159	45	.915	9.145	1.989	1.00	13.50	A
10	ATOM	735	CA	LEU A			.191	9.340	3.241		15.20	А
10												
	ATOM	736	СВ	LEU A			.031	10.835	3.517		14.20	A
	ATOM	737	CG	LEU A	159	46.	.270	11.726	3.385	1.00	19.00	A
	ATOM	738	CD1	LEU A	159	45	.847	13.188	3.477	1.00	17.12	A
	ATOM	739		LEU A			.275	11.390	4.471		14.71	А
1.5												
15	ATOM	740	С	LEU A			.809	8.716	3.232		15.53	A
	MOTA	741	0	LEU A	159	43.	.232	8.472	2.177	1.00	16.05	A
	ATOM	742	N	SER A	160	43.	.268	8.469	4.418	1.00	15.86	A
	ATOM	743	CA	SER A	160	41	.932	7.917	4.498	1.00	19.01	A
		744	CB	SER A			.566	7.582	5.949		22.90	
20	ATOM											A
20	MOTA	745	OG	SER A		4 1	.901	8.629	6.833		24.18	A
	ATOM	746	С	SER A	160	40.	.987	8.968	3.924	1.00	20.43	A
	ATOM	747	0	SER A	160	41.	.213	10.173	4.062	1.00	19.96	A
	ATOM	748	N	TYR A			.945	8.508	3.250		19.20	A
	ATOM	749	CA	TYR A			.975	9.406	2.644		20.37	A
25	ATOM	750	СВ	TYR A	161	38.	.471	8.785	1.332	1.00	20.00	A
	ATOM	751	CG	TYR A	161	37.	.314	9.502	0.666	1.00	20.72	A
	ATOM	752	CD1	TYR A	161	37	.222	10.895	0.682	1 00	18.22	А
		753						11.557	0.029		22.24	
	ATOM			TYR A			.180					A
	MOTA	754		TYR A		36.	.333	8.784	-0.020		20.53	A
30	ATOM	755	CE2	TYR A	161	35.	.287	9.436	-0.678	1.00	24.24	A
	ATOM	756	CZ	TYR A	161	35.	.218	10.822	-0.648	1.00	22.32	A
	ATOM	757	OH	TYR A			.194	11.471	-1.298		23.03	A
	MOTA	758	С	TYR A			.812	9.681	3.598		20.14	A
	ATOM	759	0	TYR A	161	36.	.959	8.819	3.810	1.00	19.53	A
35	ATOM	760	N	ALA A	162	37.	.791	10.880	4.178	1.00	19.92	A
	ATOM	761	CA	ALA A	162	36	.721	11.271	5.099	1 00	21.07	A
		762		ALA A				12.419	6.002		19.60	
	ATOM		СВ				.187					A
	MOTA	763	С	ALA A	162	35.	.542	11.712	4.238		22.07	A
	ATOM	764	0	ALA A	162	35.	.436	12.875	3.860	1.00	20.66	A
40	ATOM	765	N	LYS A	163	34	.653	10.769	3.945	1.00	23.27	A
	ATOM	766	CA	LYS A			.503	11.017	3.080		27.12	А
	ATOM	767	СВ	LYS A			.663	9.741	2.963		29.68	A
	MOTA	768	CG	LYS A	163		.455	8.524	2.515		37.67	A
	ATOM	769	CD	LYS A	163	32.	.556	7.310	2.321	1.00	42.24	A
45	ATOM	770	CE	LYS A	163	33.	.373	6.034	2.185	1.00	44.48	А
	ATOM	771	NZ	LYS A			.143	5.735	3.430		44.88	
												A
	MOTA	772	С	LYS A	163		.581	12.186	3.411		25.78	A
	MOTA	773	0	LYS A	163	32.	.103	12.863	2.506	1.00	26.53	A
	ATOM	774	N	ASN A	164	32	.327	12.441	4.689	1.00	24.57	A
50	ATOM	775	CA	ASN A			.420	13.522	5.033		23.77	А
50												
	ATOM	776	СВ	ASN A			.610	13.129	6.265		25.02	A
	ATOM	777	CG	ASN A	164	29.	.537	12.101	5.932	1.00	27.54	A
	ATOM	778	OD1	ASN A	164	28.	.772	12.281	4.983	1.00	28.79	A
	ATOM	779		ASN A			.475	11.024	6.704		27.13	A
55												
55	ATOM	780	С	ASN A			.999	14.931	5.169		24.43	A
	MOTA	781	0	ASN A	164	31	.306	15.856	5.589	1.00	23.98	A
	ATOM	782	N	GLY A	165	33	.262	15.097	4.795	1.00	21.56	A
	ATOM	783	CA	GLY A			.873	16.414	4.836		24.39	А
	ATOM	784	C	GLY A			.191	17.043	6.181		23.62	A
	AIOM	104	C	о пі <i>Р</i>	7 700	34	. <u></u>	17.043	0.101	т.00	43.64	А

	ATOM	785	0	GLY	Α	165	34.380	16.352	7.177	1.00	23.26	A
		786		GLU				18.373			23.22	
	ATOM		N				34.234		6.186			A
	ATOM	787	ca	GLU	Α	166	34.563	19.176	7.362	1.00	24.54	A
	ATOM	788	СВ	GLU	Δ	166	35.055	20.558	6.913	1 00	25.04	A
_												
5	ATOM	789	CG	GLU			36.419	20.569	6.229		26.48	A
	ATOM	790	CD	GLU	Α	166	36.699	21.889	5.517	1.00	30.02	A
	ATOM	791	OE 1	GLU	Ζ	166	36.081	22.906	5.889	1 00	29.33	А
	ATOM	792	OE2	GLU	Α	166	37.544	21.916	4.596	1.00	30.48	A
	ATOM	793	С	GLU	Α	166	33.436	19.372	8.369	1.00	24.44	A
10	ATOM	794	0	GLU			32.279	19.541	8.001		22.76	А
10												
	ATOM	795	N	LEU	Α	167	33.791	19.370	9.649	1.00	22.95	A
	ATOM	796	CA	LEU	Α	167	32.813	19.581	10.707	1.00	22.26	A
		797		LEU			33.497				22.32	
	ATOM		СВ					19.481	12.073			A
	ATOM	798	CG	LEU	Α	167	32.706	19.923	13.306	1.00	22.04	A
15	ATOM	799	CD1	LEU	Α	167	31.454	19.074	13.463	1.00	19.66	А
10												
	ATOM	800		LEU			33.597	19.805	14.537		21.17	A
	ATOM	801	С	LEU	Α	167	32.193	20.971	10.529	1.00	23.49	A
	ATOM	802	0	LEU	Δ	167	31.047	21.209	10.907	1 00	23.56	А
	ATOM	803	N	LEU			32.960	21.887	9.948		24.25	A
20	ATOM	804	CA	LEU	Α	168	32.473	23.245	9.722	1.00	26.64	A
	ATOM	805	СВ	LEU	7	168	33.560	24.099	9.066	1 00	25.62	А
	ATOM	806	CG	LEU	Α	168	33.198	25.546	8.707		27.34	A
	ATOM	807	CD1	LEU	Α	168	32.718	26.296	9.946	1.00	26.42	A
	ATOM	808		LEU			34.418	26.238	8.119		26.74	A
25	ATOM	809	С	LEU	Α	168	31.234	23.218	8.829	1.00	27.13	A
	ATOM	810	0	LEU	Α	168	30.297	23.989	9.030	1.00	26.01	A
				LYS								
	ATOM	811	N				31.233	22.320	7.848		26.41	A
	ATOM	812	ca	$_{ m LYS}$	Α	169	30.106	22.210	6.934	1.00	27.70	A
	ATOM	813	СВ	LYS	Δ	169	30.324	21.064	5.945	1.00	30.49	А
20												
30	ATOM	814	CG	LYS			29.151	20.854	4.993		32.47	A
	ATOM	815	CD	LYS	Α	169	29.407	19.728	3.998	1.00	35.98	A
	ATOM	816	CE	LYS	Δ	169	29.462	18.372	4.683	1 00	38.53	A
	ATOM	817	NZ	LYS	Α	169	29.622	17.263	3.702		41.00	A
	ATOM	818	С	LYS	Α	169	28.801	21.985	7.682	1.00	28.12	A
35	ATOM	819	0	LYS	Δ	169	27.785	22.608	7.371		28.08	А
55												
	ATOM	820	N	TYR	А	1/0	28.826	21.094	8.668	1.00	26.53	A
	ATOM	821	CA	TYR	Α	170	27.624	20.791	9.434	1.00	26.95	A
	ATOM	822	СВ	TYR	7\	170	27.810	19.476	10.193	1 00	25.03	А
	ATOM	823	CG	TYR	Α	1/0	27.898	18.300	9.251		26.65	A
40	ATOM	824	CD1	TYR	Α	170	26.745	17.661	8.790	1.00	28.27	A
	ATOM	825	CE1	TYR	Δ	170	26.814	16.642	7.839	1 00	26.85	А
	ATOM	826	CD2	TYR	Α	1/0	29.127	17.884	8.742		27.83	A
	ATOM	827	CE2	TYR	Α	170	29.209	16.869	7.792	1.00	27.19	A
	ATOM	828	CZ	TYR	Ζ	170	28.049	16.254	7.343		30.02	А
4.5												
45	ATOM	829	OH	TYR	А	1/0	28.130	15.268	6.382	1.00	29.23	A
	ATOM	830	С	TYR	Α	170	27.229	21.918	10.376	1.00	27.59	A
	ATOM	831	0	TYR	7\	170	26.045	22.122	10.642		29.25	A
	ATOM	832	Ν	ILE	Α	171	28.208	22.660	10.882	1.00	28.16	A
	ATOM	833	CA	ILE	Α	171	27.883	23.770	11.763	1.00	29.03	A
50	ATOM	834	СВ	ILE			29.151	24.435	12.337		27.51	A
50												
	ATOM	835	CG2	ILE	Α	171	28.773	25.705	13.084	1.00	27.97	A
	ATOM	836	CG1	ILE	Α	171	29.872	23.458	13.272	1.00	26.70	А
	ATOM	837		ILE			31.163	23.996	13.856		24.07	A
	ATOM	838	С	ILE	Α	171	27.094	24.796	10.944	1.00	31.41	A
55	ATOM	839	0	ILE	Α	171	26.088	25.335	11.407	1.00	31.69	A
	ATOM	840	N	ARG			27.546	25.047	9.719		33.21	A
	ATOM	841	CA	ARG	Α	172	26.874	26.000	8.844	1.00	36.54	А
	ATOM	842	СВ	ARG	Α	172	27.734	26.314	7.616	1.00	37.73	A
	ATOM	843	CG	ARG	А	1/4	29.057	27.011	7.912	T.00	41.65	А

	ATOM	844	CD	ARG	A	172	29.708	27.492	6.616	1.00	45.29	А
	ATOM	845	NE	ARG	Α	172	31.037	28.070	6.812	1.00	48.51	А
	ATOM	846	CZ	ARG	A	172	31.314	29.059	7.658	1.00	51.53	A
	ATOM	847	NH1	ARG	Α	172	30.355	29.593	8.406	1.00	53.75	A
5	ATOM	848	NH2	ARG	Α	172	32.553	29.526	7.748	1.00	51.21	A
	ATOM	849	С	ARG	Α	172	25.528	25.459	8.378	1.00	37.67	A
	ATOM	850	0	ARG	Α	172	24.550	26.200	8.288	1.00	39.09	A
	ATOM	851	N	LYS	Α	173	25.481	24.163	8.092	1.00	38.44	A
	ATOM	852	CA	LYS	Α	173	24.259	23.528	7.619	1.00	39.25	A
10	ATOM	853	СВ	LYS	Α	173	24.523	22.061	7.272	1.00	41.89	A
	ATOM	854	CG			173	23.279	21.298	6.830		45.52	A
	ATOM	855	CD	LYS			23.557	19.808	6.653		49.60	A
	ATOM	856	CE			173	24.477	19.530	5.469		52.63	A
	ATOM	857	NZ			173	23.855	19.894	4.160		54.61	A
15	ATOM	858	С			173	23.089	23.608	8.595		39.30	A
	ATOM	859	0			173	21.981	23.960	8.201		39.62	A
	ATOM	860	N			174	23.320	23.282	9.863		37.96	A
	ATOM	861	CA			174	22.229	23.314	10.833		37.36	A
20	ATOM	862	СВ			174	22.159	21.998	11.652		37.44	A
20	ATOM	863		ILE			22.058	20.802	10.709		38.37	A
	ATOM	864		ILE			23.397	21.850	12.532		37.25	A
	ATOM	865	CD1				23.355	20.620	13.418		36.85	A
	ATOM	866	C			174	22.259	24.492	11.801		36.71	A
25	ATOM	867	0			174	21.448	24.556	12.724		38.05	A
25	ATOM	868	N			175	23.185	25.423	11.592		35.48	A
	ATOM	869	CA			175	23.265	26.585	12.462		35.29	A
	MOTA	870 971	C			175 175	24.053 25.066	26.360	13.737		35.06 37.46	A
	MOTA	871 872	O N			176	23.581	27.019 25.441	13.970 14.571		33.94	A A
30	ATOM ATOM	873	CA			176	24.253	25.441	15.822		32.84	A
30	ATOM	874	CB			176	23.938	26.155	16.901		33.54	A
	ATOM	875	OG			176	22.599	26.056	17.347		34.86	A
	ATOM	876	C			176	23.796	23.731	16.276		32.34	A
	ATOM	877	0			176	22.726	23.263	15.884		32.82	A
35	ATOM	878	N			177	24.609	23.085	17.103		29.39	A
	ATOM	879	CA			177	24.313	21.743	17.597		27.20	A
	ATOM	880	СВ			177	25.621	20.989	17.865		26.39	A
	ATOM	881	CG			177	26.372	20.585	16.622		26.18	A
	ATOM	882		PHE			26.210	21.277	15.426		25.30	A
40	ATOM	883		PHE			27.266	19.516	16.662		26.05	А
	ATOM	884	CE1	PHE	Α	177	26.923	20.912	14.290	1.00	26.59	А
	ATOM	885	CE2	PHE	Α	177	27.986	19.143	15.532	1.00	26.06	A
	ATOM	886	CZ	PHE	Α	177	27.815	19.841	14.343	1.00	25.42	A
	ATOM	887	С	PHE	Α	177	23.500	21.752	18.884	1.00	27.00	A
45	ATOM	888	0	PHE	Α	177	23.704	22.610	19.747	1.00	26.48	A
	ATOM	889	N	ASP	A	178	22.578	20.802	19.022	1.00	26.70	A
	ATOM	890	CA	ASP	Α	178	21.816	20.729	20.260	1.00	26.35	A
	ATOM	891	СВ	ASP	Α	178	20.621	19.773	20.142	1.00	29.90	A
	ATOM	892	CG	ASP			21.020	18.372	19.720		32.28	A
50	ATOM	893		ASP			22.157	17.949	20.014		35.21	A
	ATOM	894		ASP			20.179	17.683	19.105		34.79	A
	ATOM	895	С	ASP			22.810	20.228	21.311		25.03	А
	ATOM	896	0	ASP			23.974	19.968	20.992		21.24	A
	ATOM	897	N			179	22.361	20.083	22.552		23.60	A
55	ATOM	898	CA	GLU			23.247	19.644	23.619		25.18	A
	ATOM	899	СВ			179	22.542	19.770	24.971		27.60	A
	ATOM	900	CG	GLU			23.324	19.176	26.130		32.58	A
	ATOM	901	CD OD 1			179	22.997	19.845	27.449		35.82	A
	ATOM	902	OET	GLU	А	т/9	21.825	20.224	27.645	T.00	35.95	A

	ATOM	903	OE2	GLU A	179	23.912	19.984	28.291	1.00 38.19	A
	ATOM	904	С	GLU A	179	23.808	18.235	23.450	1.00 24.08	A
	ATOM	905	0	GLU A		24.977	17.989	23.756	1.00 22.79	A
	ATOM	906	N	THR A		22.983		22.961	1.00 23.36	A
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5	MOTA	907	CA	THR A		23.412	15.935	22.761	1.00 22.15	A
	ATOM	908	СВ	THR A		22.224		22.320	1.00 23.77	A
	MOTA	909	0G1	THR A	180	21.222	15.075	23.341	1.00 26.37	A
	ATOM	910	CG2	THR A	180	22.670	13.616	22.088	1.00 22.66	A
	ATOM	911	С	THR A	180	24.533	15.830	21.724	1.00 22.01	A
10	ATOM	912	0	THR A		25.533		21.944	1.00 19.87	А
• •	ATOM	913	N	CYS A		24.365		20.596	1.00 21.21	A
	ATOM	914	CA	CYS A		25.372		19.541	1.00 22.22	A
	ATOM	915	CB	CYS A		24.800		18.250	1.00 24.62	A
	ATOM	916	SG	CYS A		23.435		17.560	1.00 29.50	A
15	ATOM	917	С	CYS A		26.633		19.954	1.00 23.07	A
	ATOM	918	0	CYS A	181	27.746	16.827	19.608	1.00 23.95	A
	MOTA	919	N	THR A	182	26.463	18.325	20.695	1.00 22.76	A
	MOTA	920	CA	THR A	182	27.606	19.103	21.161	1.00 21.49	A
	ATOM	921	СВ	THR A	182	27.167	20.346	21.978	1.00 21.37	А
20	ATOM	922	0G1	THR A	182	26.459		21.134	1.00 22.50	А
	ATOM	923		THR A		28.379		22.565	1.00 18.36	A
	ATOM	924	C	THR A		28.454		22.071	1.00 21.48	
										A
	ATOM	925	0	THR A		29.669	18.090	21.894	1.00 19.95	A
	ATOM	926	N	ARG A		27.798		23.050	1.00 18.97	A
25	MOTA	927	CA	ARG A	183	28.468	16.723	23.996	1.00 19.39	A
	MOTA	928	СВ	ARG A	183	27.455	16.140	24.984	1.00 19.46	A
	ATOM	929	CG	ARG A	183	28.030	15.062	25.887	1.00 18.77	A
	ATOM	930	CD	ARG A	183	27.021	14.571	26.925	1.00 21.19	A
	ATOM	931	NE	ARG A		26.605		27.824	1.00 19.46	А
30	ATOM	932	CZ	ARG A		25.496		27.679	1.00 20.45	A
30	ATOM	933		ARG A		24.672	16.123	26.666	1.00 20.45	A
	ATOM	934		ARG A		25.224	17.338	28.539	1.00 17.11	A
	ATOM	935	С	ARG A		29.206		23.302	1.00 20.02	A
	MOTA	936	0	ARG A	183	30.383		23.573	1.00 19.97	A
35	MOTA	937	N	PHE A	184	28.520	14.871	22.409	1.00 19.24	A
	MOTA	938	CA	PHE A	184	29.144	13.746	21.722	1.00 18.04	A
	ATOM	939	СВ	PHE A	184	28.158	13.078	20.764	1.00 21.05	A
	ATOM	940	CG	PHE A	184	28.719	11.857	20.098	1.00 22.67	A
	ATOM	941	CD1	PHE A	184	28.717		20.754	1.00 22.97	A
40	ATOM	942		PHE A		29.317		18.850	1.00 19.97	A
.0	ATOM	943		PHE A		29.308	9.510	20.176	1.00 23.53	A
								18.263		_
	ATOM	944		PHE A		29.915			1.00 24.11	A
	ATOM	945	CZ	PHE A		29.910		18.928	1.00 22.97	A
	MOTA	946	С	PHE A		30.403		20.941	1.00 17.99	A
45	ATOM	947	0	PHE A	184	31.461		21.130	1.00 18.89	A
	MOTA	948	N	TYR A	185	30.292	15.110	20.056	1.00 15.73	A
	MOTA	949	CA	TYR A	185	31.443	15.519	19.265	1.00 15.72	A
	ATOM	950	СВ	TYR A	185	30.992	16.413	18.111	1.00 17.33	A
	ATOM	951	CG	TYR A		30.364		17.015	1.00 19.37	А
50	ATOM	952		TYR A		31.159		16.168	1.00 16.53	A
50	ATOM	953		TYR A		30.590		15.232	1.00 18.12	A
	ATOM	954		TYR A		28.976		16.892	1.00 18.18	A
	ATOM	955		TYR A		28.398		15.956	1.00 18.90	A
	ATOM	956	CZ	TYR A		29.211		15.133	1.00 18.41	A
55	ATOM	957	OH	TYR A		28.650		14.218	1.00 20.48	A
	ATOM	958	С	TYR A	185	32.544	16.172	20.083	1.00 15.79	A
	ATOM	959	0	TYR A	185	33.720	16.015	19.766	1.00 17.69	A
	ATOM	960	N	THR A		32.176		21.142	1.00 15.68	А
	ATOM	961	CA	THR A		33.184		21.997	1.00 16.03	A
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	ATOM	962	СВ	THR	Α	186	32.559	18.403	23.094	1.00	16.62	А
	ATOM	963	OG1	THR	Α	186	31.866	19.503	22.481	1.00	14.79	А
	ATOM	964	CG2	THR	Α	186	33.656	18.953	24.019	1.00	14.68	A
	ATOM	965	С	THR	Α	186	33.954	16.375	22.680	1.00	15.59	A
5	ATOM	966	0	THR	Α	186	35.176	16.443	22.823	1.00	13.77	A
	ATOM	967	N	ALA	Α	187	33.234	15.333	23.097	1.00	14.06	A
	ATOM	968	CA	ALA	Α	187	33.869	14.196	23.757	1.00	14.74	A
	ATOM	969	СВ	ALA	Α	187	32.810	13.195	24.224	1.00	14.32	A
	ATOM	970	C	ALA	Α	187	34.875	13.509	22.821	1.00	14.41	A
10	ATOM	971	0	ALA	Α	187	35.972	13.136	23.247	1.00	15.61	A
	ATOM	972	N	GLU	Α	188	34.516	13.340	21.549	1.00	14.01	A
	ATOM	973	CA	GLU	Α	188	35.443	12.704	20.615	1.00	13.50	A
	ATOM	974	СВ	GLU	Α	188	34.782	12.449	19.251	1.00	12.85	A
	ATOM	975	CG	GLU	Α	188	33.622	11.454	19.282		12.71	A
15	ATOM	976	CD	GLU			33.464	10.685	17.979		15.01	A
	ATOM	977		GLU			33.687	11.275	16.899		13.21	A
	ATOM	978	OE2	GLU	Α	188	33.110	9.484	18.031	1.00	17.69	A
	ATOM	979	С	GLU	Α	188	36.682	13.582	20.436		13.34	A
	ATOM	980	0	GLU			37.803	13.085	20.408		14.69	A
20	ATOM	981	N	ILE			36.486	14.893	20.326		13.52	A
	ATOM	982	CA	ILE			37.627	15.787	20.159		13.35	A
	ATOM	983	СВ	ILE			37.169	17.247	19.939		13.95	А
	ATOM	984		ILE			38.381	18.165	19.822		12.47	А
	ATOM	985		ILE			36.302	17.332	18.671		13.44	A
25	ATOM	986		ILE			35.588	18.664	18.491		14.29	A
	ATOM	987	С	ILE			38.530	15.702	21.394		14.63	A
	ATOM	988	0	ILE			39.753	15.595	21.271		12.97	A
	ATOM	989	N	VAL			37.927	15.751	22.582		14.35	A
20	ATOM	990	CA	VAL			38.684	15.655	23.832		13.22	A
30	ATOM	991	CB	VAL			37.743	15.690	25.061		14.28	A
	ATOM	992		VAL			38.509	15.267	26.326		15.08	A
	ATOM	993	CG2				37.160	17.082	25.233		12.08	A
	ATOM	994	C	VAL			39.468	14.338	23.859		14.61	A
25	ATOM	995	O	VAL			40.634	14.304	24.250		13.72	A
35	ATOM	996	N	SER			38.825	13.254	23.432		15.26	A
	ATOM	997	CA	SER		191	39.478	11.943	23.421		16.81	A
	ATOM	998 999	CB OG	SER			38.470	10.857 9.569	23.041		16.14	A
	ATOM ATOM	1000	C	SER			39.018 40.649	11.928	23.238 22.441		16.94 16.58	A A
40	ATOM	1000	0	SER			41.697	11.335	22.713		13.96	A
40	ATOM	1001	N	ALA			40.468	12.586	21.300		15.26	A
	ATOM	1002	CA	ALA			41.518	12.645	20.292		14.37	A
	ATOM	1003	CB	ALA			40.989	13.296	19.016		14.43	A
	ATOM	1005	C	ALA			42.695	13.440	20.845		16.46	A
45	ATOM	1006	0	ALA			43.851	13.038	20.697		17.96	A
15	ATOM	1007	N	LEU			42.401	14.563	21.496		15.02	A
	ATOM	1008	CA	LEU			43.459	15.392	22.067		15.42	A
	ATOM	1009	СВ	LEU			42.884	16.712	22.600		12.88	A
	ATOM	1010	CG	LEU			42.445	17.721	21.525		15.97	A
50	ATOM	1011		LEU			41.869	18.979	22.190		13.97	А
	ATOM	1012		LEU			43.642	18.088	20.655		14.58	А
	ATOM	1013	С	LEU			44.211	14.659	23.174	1.00	14.49	А
	ATOM	1014	0	LEU			45.427	14.813	23.310		16.56	А
	ATOM	1015	N	GLU			43.500	13.870	23.975		13.96	А
55	ATOM	1016	CA	GLU	А	194	44.179	13.123	25.032	1.00	14.08	A
	ATOM	1017	СВ	GLU			43.190	12.295	25.857		14.65	А
	ATOM	1018	CG	GLU	А	194	43.882	11.301	26.789	1.00	17.09	А
	ATOM	1019	CD	GLU			42.924	10.592	27.730		19.59	A
	MOTA	1020	OE1	GLU	Α	194	41.809	10.237	27.295	1.00	19.25	A

	ATOM	1021	OE2	GLU			43.302	10.380	28.906	1.00 20.20	A
	ATOM	1022	С	GLU			45.208	12.199	24.386	1.00 13.57	
	ATOM	1023	0	GLU			46.337	12.093	24.847	1.00 14.23	
-	ATOM	1024	N	TYR			44.822	11.544	23.301	1.00 14.89	A
5	ATOM	1025	CA	TYR			45.743	10.642	22.618	1.00 16.58	A
	ATOM	1026	CB	TYR			45.030	9.910	21.488	1.00 17.29	A
	ATOM	1027	CG			195	45.956	9.058	20.649	1.00 17.92	
	ATOM	1028		TYR			46.347	7.788	21.077	1.00 17.96	
10	ATOM	1029		TYR			47.203	6.996	20.304	1.00 19.77	
10	ATOM	1030	CD2				46.445	9.524	19.428	1.00 16.67	A
	ATOM	1031	CE2				47.299	8.744	18.650	1.00 18.51	
	ATOM	1032	CZ	TYR			47.671	7.481	19.094	1.00 20.24	A
	ATOM	1033	OH	TYR			48.506	6.705	18.325	1.00 21.89	A
15	ATOM	1034	C	TYR			46.917	11.419	22.035	1.00 16.98	A
15	ATOM	1035	O N	TYR			48.081	11.047	22.203	1.00 14.61	
	ATOM	1036	N	LEU			46.599	12.507	21.347	1.00 16.30	
	ATOM	1037 1038	CA	LEU			47.619	13.328 14.502	20.720	1.00 18.15	
	ATOM	1030	CB CG	LEU LEU			46.969 47.834	15.203	19.982 18.935	1.00 18.59 1.00 22.51	
20	ATOM ATOM	1039		LEU			48.222	14.206	17.841	1.00 22.31	A A
20	ATOM	1040		LEU			47.060	16.375	18.338	1.00 20.94	A
	ATOM	1041	CD2	LEU			48.592	13.844	21.763	1.00 22.98	
	ATOM	1042	0	LEU			49.801	13.644	21.763	1.00 17.73	
	ATOM	1043	N	HIS			48.064	14.495	22.792	1.00 10.33	A
25	ATOM	1044	CA	HIS			48.913	15.042	23.842	1.00 17.12	A
23	ATOM	1045	CB	HIS			48.069	15.866	24.817	1.00 15.90	A
	ATOM	1047	CG	HIS			47.571	17.152	24.231	1.00 19.15	
	ATOM	1047		HIS			47.830	17.745	23.038	1.00 19.13	A
	ATOM	1049		HIS			46.704	17.743	24.897	1.00 17.47	A
30	ATOM	1050		HIS			46.450	19.047	24.139	1.00 17.47	A
30	ATOM	1050		HIS			47.119	18.921	23.007	1.00 15.69	A
	ATOM	1052	C	HIS			49.696	13.958	24.572	1.00 19.40	A
	ATOM	1053	0	HIS			50.823	14.192	25.021	1.00 19.42	A
	ATOM	1054	N	GLY			49.106	12.770	24.679	1.00 18.59	
35	ATOM	1055	CA	GLY			49.793	11.675	25.339	1.00 19.60	A
00	ATOM	1056	C	GLY			51.075	11.307	24.612	1.00 21.86	
	ATOM	1057	0	GLY			51.963	10.682	25.186	1.00 23.09	
	ATOM	1058	N	LYS			51.174	11.687	23.341	1.00 22.81	
	ATOM	1059	CA	LYS			52.368	11.401	22.549	1.00 24.43	A
40	ATOM	1060	СВ	LYS			51.990	10.905	21.154	1.00 26.00	А
	ATOM	1061	CG	LYS			51.378	9.520	21.133	1.00 30.98	A
	ATOM	1062	CD	LYS	Α	199	51.291	9.002	19.708	1.00 36.85	А
	ATOM	1063	CE	LYS	Α	199	50.832	7.559	19.682	1.00 40.37	А
	ATOM	1064	NΖ	LYS	Α	199	51.646	6.691	20.581	1.00 43.48	A
45	ATOM	1065	С	LYS	Α	199	53.253	12.631	22.414	1.00 23.88	A
	ATOM	1066	0	LYS			54.144	12.669	21.568	1.00 24.97	А
	ATOM	1067	N	GLY	Α	200	52.997	13.638	23.243	1.00 24.00	A
	ATOM	1068	CA	GLY	Α	200	53.790	14.853	23.203	1.00 22.12	A
	ATOM	1069	С	GLY	Α	200	53.665	15.632	21.907	1.00 22.14	A
50	ATOM	1070	0	GLY	Α	200	54.632	16.231	21.439	1.00 22.41	A
	ATOM	1071	N	ILE	Α	201	52.475	15.630	21.320	1.00 20.00	A
	ATOM	1072	CA	ILE	Α	201	52.252	16.355	20.080	1.00 18.93	A
	ATOM	1073	СВ	ILE	A	201	51.784	15.414	18.955	1.00 19.70	A
	ATOM	1074	CG2	ILE	Α	201	51.414	16.226	17.716	1.00 20.12	A
55	ATOM	1075		ILE			52.880	14.395	18.636	1.00 20.03	A
	MOTA	1076	CD1	ILE			52.408	13.258	17.745	1.00 22.75	A
	ATOM	1077	С			201	51.193	17.425	20.270	1.00 19.87	A
	ATOM	1078	0			201	50.121	17.161	20.817	1.00 20.08	A
	MOTA	1079	N	ILE	Α	202	51.508	18.633	19.815	1.00 19.94	A

	ATOM	1080	CA	ILE	Α	202	50.601	19.772	19.891	1.00	20.45	A
	ATOM	1081	СВ	ILE	Ζ	202	51.352	21.040	20.356	1 00	22.21	А
	ATOM	1082		ILE			50.381	22.220	20.470		22.67	A
	MOTA	1083	CG1	ILE	Α	202	52.033	20.775	21.700	1.00	24.19	A
5	ATOM	1084	CD1	ILE	Δ	202	52.914	21.920	22.169	1 00	25.39	A
,												
	ATOM	1085	С	ILE			50.105	19.999	18.464		20.71	A
	MOTA	1086	0	ILE	Α	202	50.910	20.067	17.538	1.00	19.48	A
	ATOM	1087	N	HIS	Α	203	48.795	20.108	18.270	1.00	18.65	A
	ATOM	1088	CA	HIS			48.280	20.319	16.919		18.02	A
1.0												
10	ATOM	1089	СВ	HIS			46.775	20.057	16.874	1.00	16.31	A
	ATOM	1090	CG	HIS	Α	203	46.199	20.136	15.495	1.00	18.36	A
	ATOM	1091	CD2	HIS	Δ	203	46.043	21.186	14.655	1.00	16.42	А
	ATOM	1092		HIS			45.759	19.026	14.806		19.50	A
	MOTA	1093	CE1	HIS	Α	203	45.359	19.389	13.600	1.00	17.64	A
15	ATOM	1094	NE2	HIS	Α	203	45.522	20.694	13.483	1.00	20.87	A
	ATOM	1095	С	HIS	Δ	203	48.589	21.738	16.405	1 00	18.92	А
	ATOM	1096	0	HIS			49.073	21.906	15.282		16.21	А
	MOTA	1097	N	ARG	Α	204	48.301	22.744	17.232	1.00	18.60	A
	ATOM	1098	CA	ARG	Α	204	48.552	24.157	16.914	1.00	19.81	А
20	ATOM	1099	СВ	ARG			49.998	24.365	16.458		21.61	A
20												
	ATOM	1100	CG	ARG	А	204	51.024	24.137	17.550		23.82	A
	MOTA	1101	CD	ARG	Α	204	52.323	24.870	17.252	1.00	27.62	A
	ATOM	1102	NE	ARG	Α	204	52.932	24.449	15.994	1.00	29.43	А
							54.125					
	ATOM	1103	CZ	ARG				24.861	15.572		33.10	А
25	MOTA	1104	NH1	ARG	Α	204	54.835	25.706	16.311	1.00	32.12	A
	ATOM	1105	NH2	ARG	Α	204	54.614	24.426	14.418	1.00	30.25	A
	ATOM	1106	С	ARG	Δ	204	47.624	24.830	15.905	1 00	20.03	А
	ATOM	1107	0	ARG			47.711	26.038	15.698		20.88	A
	ATOM	1108	N	ASP	Α	205	46.755	24.071	15.255	1.00	18.96	A
30	ATOM	1109	CA	ASP	Α	205	45.828	24.692	14.325	1.00	17.90	A
	ATOM	1110	СВ	ASP			46.418	24.741	12.914		18.95	A
	ATOM	1111	CG	ASP			45.655	25.688	12.008		20.36	A
	ATOM	1112	OD1	ASP	Α	205	44.939	26.560	12.545	1.00	20.35	A
	ATOM	1113	OD2	ASP	Α	205	45.772	25.573	10.771	1.00	22.49	A
35	ATOM	1114	C	ASP			44.500	23.956	14.328		19.60	A
33												
	ATOM	1115	0	ASP			43.876	23.751	13.287	1.00	21.53	A
	ATOM	1116	N	LEU	Α	206	44.063	23.569	15.521	1.00	18.53	A
	ATOM	1117	CA	LEU	Ά	206	42.813	22.851	15.667	1.00	19.18	A
	ATOM	1118	СВ	LEU			42.693	22.295	17.087		18.94	A
40												
40	MOTA	1119	CG	LEU			41.511	21.358	17.346		23.10	A
	ATOM	1120	CD1	LEU	Α	206	41.615	20.142	16.436	1.00	23.01	A
	ATOM	1121	CD2	LEU	Ά	206	41.504	20.933	18.808	1.00	22.97	A
	ATOM	1122		LEU			41.639	23.772	15.361		19.05	
			С									A
	MOTA	1123	0	LEU	Α	206	41.556	24.880	15.886	1.00	19.25	A
45	ATOM	1124	N	LYS	Α	207	40.740	23.307	14.500	1.00	17.54	A
	ATOM	1125	CA	LYS	Δ	207	39.564	24.081	14.110		18.60	А
	ATOM	1126	СВ	LYS			39.980	25.248	13.196		18.98	A
	MOTA	1127	CG	LYS	Α	207	40.786	24.817	11.982	1.00	18.20	A
	MOTA	1128	CD	LYS	Α	207	41.246	26.000	11.139	1.00	21.42	A
50	ATOM	1129	CE	LYS			42.223	25.537	10.062		23.21	А
50												
	ATOM	1130	NZ	LYS			42.561	26.604	9.084		29.61	А
	MOTA	1131	С	LYS	Α	207	38.566	23.181	13.388	1.00	18.18	A
	ATOM	1132	0	LYS	Α	207	38.921	22.100	12.915	1.00	18.11	А
	ATOM	1133	N	PRO			37.298	23.614	13.293		20.26	A
55	ATOM	1134	CD	PRO			36.713	24.833	13.882		18.79	А
	ATOM	1135	CA	PRO	Α	208	36.272	22.814	12.616	1.00	19.67	A
	ATOM	1136	СВ	PRO	Α	208	35.063	23.742	12.608		19.45	A
	ATOM	1137	CG	PRO			35.231	24.509	13.891		21.81	A
	ATOM	1138	С	PRO	А	ZUB	36.674	22.372	11.209	T.00	21.04	A

	ATOM	1139	0	PRO	Α	208	36.264	21.307	10.751	1.00	21.19	A
	ATOM	1110		GLU			37.474					
		1140	N					23.188	10.528		21.69	А
	MOTA	1141	ca	GLU	Α	209	37.928	22.872	9.170	1.00	22.64	A
	ATOM	1142	СВ	GLU	Δ	209	38.644	24.084	8.558	1 00	23.65	А
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5	ATOM	1143	CG	GLU			39.253	23.825	7.185		27.24	A
	ATOM	1144	CD	GLU	Α	209	40.155	24.958	6.716	1.00	29.40	A
	ATOM	1145	OF 1	GLU	7\	200	39.660	26.094	6.553	1 00	29.68	А
	MOTA	1146	OE2	GLU	Α	209	41.363	24.711	6.511	1.00	30.07	A
	ATOM	1147	С	GLU	Α	209	38.879	21.668	9.159	1.00	22.28	A
10	ATOM	1148	0	GLU	7\	200	38.955	20.933	8.170		21.36	А
10												
	MOTA	1149	N	ASN	Α	210	39.600	21.490	10.263	1.00	19.90	A
	ATOM	1150	CA	ASN	Α	210	40.574	20.412	10.436	1.00	19.44	A
	ATOM	1151	СВ	ASN			41.744	20.912	11.287		20.07	А
	ATOM	1152	CG	ASN	Α	210	42.746	21.698	10.479	1.00	25.77	A
15	ATOM	1153	OD1	ASN	Α	210	43.571	22.427	11.029	1.00	26.73	A
	ATOM	1154		ASN			42.687	21.548	9.158		25.15	А
	ATOM	1155	С	ASN	Α	210	40.005	19.151	11.078	1.00	18.63	A
	MOTA	1156	0	ASN	Α	210	40.712	18.154	11.234	1.00	18.29	A
	ATOM	1157	N	ILE			38.739	19.202	11.469		16.31	A
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20	ATOM	1158	CA	ILE	Α	211	38.090	18.058	12.085	1.00	15.49	A
	ATOM	1159	СВ	ILE	Α	211	37.336	18.488	13.354	1.00	15.40	A
		1160		ILE			36.582	17.311	13.950		14.59	A
	ATOM											
	MOTA	1161	CG1	ILE	Α	211	38.342	19.046	14.365		15.91	A
	ATOM	1162	CD1	ILE	Α	211	37.720	19.669	15.590	1.00	15.98	А
25		1163		ILE			37.131		11.059		17.26	
23	ATOM		С					17.485				A
	MOTA	1164	0	ILE	Α	211	35.995	17.947	10.926	1.00	18.16	A
	ATOM	1165	N	LEU	Α	212	37.599	16.486	10.317	1.00	15.97	A
	ATOM	1166	CA	LEU			36.784	15.875	9.274		17.08	A
	ATOM	1167	СВ	LEU	Α	212	37.685	15.249	8.202	1.00	17.78	A
30	ATOM	1168	CG	LEU	Α	212	38.785	16.157	7.640	1.00	18.92	A
				LEU								
	ATOM	1169					39.476	15.450	6.485		22.09	А
	ATOM	1170	CD2	LEU	Α	212	38.188	17.482	7.166	1.00	19.91	A
	ATOM	1171	С	LEU	Δ	212	35.843	14.825	9.837	1 00	18.35	A
	ATOM	1172	0	LEU			35.957	14.433	11.002		19.39	A
35	ATOM	1173	N	LEU	Α	213	34.915	14.368	9.000	1.00	17.84	A
	ATOM	1174	CA	LEU	Ά	213	33.942	13.362	9.403	1.00	19.94	A
	ATOM	1175	СВ	LEU			32.556	14.004	9.487		20.84	A
	ATOM	1176	CG	$_{ m LEU}$	Α	213	32.396	15.059	10.583	1.00	20.31	A
	ATOM	1177	CD1	LEU	Α	213	31.124	15.837	10.367	1.00	22.75	A
40		1178		LEU			32.379	14.378	11.940		23.93	A
40	ATOM											
	MOTA	1179	С	LEU	Α	213	33.914	12.187	8.426	1.00	20.98	A
	MOTA	1180	0	LEU	Α	213	33.743	12.379	7.218	1.00	19.55	A
	ATOM	1181		ASN			34.088	10.970	8.935		20.44	
			N									A
	MOTA	1182	CA	ASN	Α	214	34.055	9.814	8.049	1.00	23.77	A
45	MOTA	1183	СВ	ASN	Α	214	34.745	8.596	8.674	1.00	25.30	A
	ATOM	1184	CG	ASN			34.077	8.127	9.948		32.04	
												A
	ATOM	1185	OD1	ASN	Α	214	32.908	8.422	10.206	1.00	34.43	A
	MOTA	1186	ND2	ASN	Α	214	34.818	7.369	10.752	1.00	33.85	A
	ATOM	1187	С	ASN			32.618	9.466	7.693		24.07	A
= 0												
50	MOTA	1188	0	ASN	Α	214	31.672	10.113	8.150	1.00	19.94	A
	ATOM	1189	N	GLU	Α	215	32.459	8.433	6.879	1.00	25.77	A
	ATOM	1190	CA	GLU			31.138	8.003	6.445		28.69	A
	MOTA	1191	СВ	GLU	Α	215	31.275	6.796	5.513	1.00	31.98	A
	ATOM	1192	CG	GLU	Α	215	29.970	6.334	4.896	1.00	40.22	А
55	ATOM	1193	CD	GLU			30.182	5.312	3.795		44.27	A
55												
	MOTA	1194	OE 1	GLU	Α	215	30.817	4.268	4.065	1.00	46.46	A
	MOTA	1195	OE2	GLU	Α	215	29.716	5.556	2.660	1.00	46.13	А
	ATOM	1196	C	GLU			30.188	7.673	7.601		28.41	A
	ATOM	1197	0	GLU	А	ZT2	28.971	7.769	7.447	T.00	28.52	A

	ATOM	1198	N	ASP	Α	216	30.737	7.287	8.752	1.00	26.77	A
	ATOM	1199	CA	ASP	Ζ	216	29.914	6.953	9.917	1 00	27.28	А
	MOTA	1200	СВ	ASP			30.538	5.795	10.696		31.27	A
	ATOM	1201	CG	ASP	Α	216	30.390	4.466	9.979	1.00	37.61	A
5	ATOM	1202	OD1	ASP	Δ	216	29.274	4.170	9.499	1 00	39.45	A
5												
	ATOM	1203		ASP			31.382	3.710	9.902		41.84	A
	MOTA	1204	С	ASP	Α	216	29.697	8.135	10.862	1.00	26.37	A
	ATOM	1205	0	ASP	Α	216	29.136	7.984	11.950	1.00	25.73	A
	ATOM	1206	N	MET			30.156	9.306	10.441		23.02	А
10												
10	ATOM	1207	CA	MET			30.015	10.527	11.218		21.83	A
	ATOM	1208	CB	MET	Α	217	28.537	10.789	11.517	1.00	23.24	A
	ATOM	1209	CG	MET	Α	217	27.742	11.186	10.274	1.00	22.98	А
	ATOM	1210	SD	MET			28.464	12.616	9.430		27.57	A
	MOTA	1211	CE	MET	Α	217	27.679	13.974	10.332		26.68	A
15	ATOM	1212	С	MET	Α	217	30.844	10.618	12.502	1.00	21.51	A
	ATOM	1213	0	MET	Α	217	30.474	11.323	13.440	1.00	18.62	А
	ATOM	1214	N	HIS			31.957	9.892	12.544		20.10	A
	MOTA	1215	CA	HIS	Α	218	32.873	9.964	13.678	1.00	19.86	A
	MOTA	1216	СВ	HIS	Α	218	33.482	8.594	13.977	1.00	20.21	A
20	ATOM	1217	CG	HIS	Δ	218	32.551	7.667	14.698	1.00	22.40	А
20				HIS								
	ATOM	1218					31.910	6.547	14.287		21.27	A
	MOTA	1219	ND1	HIS	Α	218	32.177	7.863	16.011	1.00	19.59	A
	MOTA	1220	CE1	HIS	Α	218	31.348	6.902	16.379	1.00	21.88	A
	ATOM	1221		HIS			31.168	6.091	15.351		22.08	А
25												
25	ATOM	1222	С	HIS			33.947	10.921	13.172		19.10	A
	MOTA	1223	0	HIS	Α	218	34.170	11.004	11.965	1.00	20.31	A
	MOTA	1224	N	ILE	Α	219	34.617	11.638	14.067	1.00	17.21	A
	ATOM	1225	CA	ILE			35.628	12.586	13.618		15.26	A
	MOTA	1226	СВ	ILE			35.987	13.614	14.716	1.00	15.38	A
30	MOTA	1227	CG2	ILE	Α	219	34.722	14.305	15.221	1.00	14.58	A
	ATOM	1228	CG1	ILE	Α	219	36.734	12.919	15.864	1.00	14.46	А
		1229		ILE			37.279	13.885			13.74	
	ATOM								16.911			A
	MOTA	1230	С	ILE	Α	219	36.929	11.944	13.161	1.00	16.21	A
	MOTA	1231	0	ILE	Α	219	37.238	10.799	13.500	1.00	15.88	A
35	ATOM	1232	N	GLN	Α	220	37.677	12.711	12.378	1.00	15.62	А
		1233		GLN			38.980	12.316			17.84	
	ATOM		CA						11.876			A
	ATOM	1234	СВ	GLN	Α	220	38.872	11.595	10.525	1.00	20.00	A
	ATOM	1235	CG	GLN	Α	220	38.463	10.129	10.659	1.00	26.97	A
	ATOM	1236	CD	GLN	Δ	220	38.648	9.343	9.372		29.95	А
40		1237		GLN			37.968	9.590	8.373		33.12	A
40	ATOM											
	MOTA	1238	NE2	GLN	Α	220	39.578	8.393	9.389	1.00	30.47	A
	MOTA	1239	С	GLN	Α	220	39.757	13.610	11.735	1.00	17.00	A
	ATOM	1240	0	GLN	Δ	220	39.609	14.339	10.751	1.00	18.27	A
	ATOM	1241		ILE			40.566	13.906	12.746		14.34	
			N									A
45	ATOM	1242	CA	ILE	Α	221	41.361	15.120	12.753	1.00	14.46	A
	MOTA	1243	СВ	ILE	Α	221	41.867	15.416	14.175	1.00	12.30	A
	ATOM	1244	CG2	ILE	Δ	221	42.764	16.656	14.167	1 00	14.78	A
	ATOM	1245		ILE			40.660	15.613	15.102		13.92	A
	MOTA	1246	CD1	ILE	Α	221	41.003	15.901	16.543	1.00	15.06	A
50	MOTA	1247	С	ILE	Α	221	42.536	14.996	11.783	1.00	15.44	A
	ATOM	1248	0	ILE			43.106	13.915	11.613		13.93	А
	ATOM	1249	N	THR			42.877	16.101	11.127		15.36	A
	MOTA	1250	CA	THR	Α	222	43.980	16.098	10.174	1.00	17.52	A
	MOTA	1251	СВ	THR	Α	222	43.470	15.836	8.750	1.00	19.92	A
55	ATOM	1252		THR			44.587	15.637	7.875		18.78	А
55												
	ATOM	1253		THR			42.630	17.018	8.257		18.16	А
	MOTA	1254	С	THR	Α	222	44.735	17.428	10.192	1.00	19.60	A
	ATOM	1255	0	THR	Α	222	44.509	18.257	11.084	1.00	18.59	A
	ATOM	1256	N	ASP			45.630	17.610	9.216		18.69	А
	211 011	1200	TA	110 L	11	225	10.000	I,.010	J. ZIV	±.00	20.00	А

	ATOM	1257	CA	ASP	Α	223	46.440	18.825	9.069	1.00	20.12	A
	7) III ()) / (1258										
	ATOM		СВ	ASP			45.532	20.065	9.108		23.51	A
	ATOM	1259	CG	ASP	Α	223	46.248	21.335	8.670	1.00	27.09	A
	ATOM	1260	OD 1	ASP	Δ	223	47.283	21.227	7.975	1 00	26.28	А
-												
5	ATOM	1261	ODZ	ASP			45.765	22.438	9.009		26.15	A
	ATOM	1262	С	ASP	Α	223	47.516	18.913	10.150	1.00	21.73	A
	ATOM	1263	0	ASP	7\	223	47.439	19.751	11.055	1 00	22.76	А
	ATOM	1264	N	PHE	Α	224	48.535	18.063	10.027	1.00	20.75	A
	ATOM	1265	CA	PHE	Α	2.2.4	49.611	17.988	11.009	1.00	20.11	A
10		1266		PHE			49.805	16.527	11.424		20.62	
10	ATOM		СВ									A
	ATOM	1267	CG	$_{ m PHE}$	Α	224	48.682	15.991	12.263	1.00	21.41	A
	ATOM	1268	CD1	PHE	Δ	224	48.598	16.312	13.614	1.00	23.05	A
	ATOM	1269		PHE			47.681	15.212	11.693		22.27	A
	ATOM	1270	CE1	PHE	Α	224	47.528	15.868	14.389	1.00	23.30	A
15	ATOM	1271	CE2	PHE	Δ	224	46.606	14.763	12.457	1 00	21.11	А
15												
	MOTA	1272	CZ	PHE			46.530	15.093	13.807		22.02	A
	ATOM	1273	С	PHE	Α	224	50.957	18.583	10.619	1.00	20.45	A
	ATOM	1274	0	PHE			51.905	18.547	11.407		20.73	А
	MOTA	1275	N	$\operatorname{GL} Y$	Α	225	51.049	19.125	9.412	1.00	22.02	A
20	ATOM	1276	CA	GLY	Α	225	52.301	19.713	8.981	1.00	22.66	A
		1277	С	GLY			52.742		9.920		24.99	
	ATOM							20.822				A
	ATOM	1278	0	$\operatorname{GL} Y$	Α	225	53.939	21.041	10.122	1.00	24.52	A
	ATOM	1279	N	THR	Δ	226	51.779	21.524	10.508	1.00	23.50	А
	ATOM	1280	CA	THR			52.106	22.613	11.416		25.16	A
25	ATOM	1281	CB	THR	Α	226	51.199	23.829	11.160	1.00	24.76	A
	ATOM	1282	∩ദ1	THR	Z \	226	49.831	23.410	11.113	1 00	22.68	А
	MOTA	1283	CG2				51.571	24.490	9.834		25.00	A
	ATOM	1284	С	THR	Α	226	52.046	22.233	12.894	1.00	25.79	A
	ATOM	1285	0	THR	7\	226	52.019	23.100	13.768	1 00	24.54	А
20												
30	ATOM	1286	N	ALA	Α	227	52.037	20.935	13.173	1.00	24.97	A
	ATOM	1287	CA	ALA	Α	227	52.004	20.475	14.550	1.00	25.49	A
	ATOM	1288	СВ	ALA			51.659	18.993	14.607		22.85	A
	ATOM	1289	С	ALA	Α	227	53.384	20.715	15.149	1.00	27.70	A
	ATOM	1290	0	ALA	A	227	54.331	21.047	14.435	1.00	26.60	A
35												
33	ATOM	1291	N	LYS			53.491	20.558	16.461		28.53	A
	ATOM	1292	CA	LYS	Α	228	54.760	20.745	17.149	1.00	32.12	A
	ATOM	1293	СВ	LYS	A	228	54.699	21.974	18.054	1.00	33.81	A
											41.23	
	ATOM	1294	CG	LYS			56.007	22.294	18.765			A
	ATOM	1295	$^{\rm CD}$	LYS	Α	228	57.082	22.725	17.768	1.00	47.57	A
40	ATOM	1296	CE	LYS	Α	228	58.401	23.056	18.462	1.00	49.82	А
	ATOM	1297	NZ	LYS			59.459	23.425	17.480		51.49	A
	ATOM	1298	С	LYS	Α	228	55.019	19.504	17.985	1.00	33.25	A
	ATOM	1299	0	LYS	A	228	54.190	19.129	18.815	1.00	33.70	A
	ATOM	1300	N	VAL			56.159	18.860	17.756		33.64	A
45	ATOM	1301	CA	VAL	Α	229	56.516	17.661	18.501	1.00	34.66	A
	ATOM	1302	СВ	VAL	Δ	229	57.248	16.646	17.609		33.50	А
	ATOM	1303	CGI	VAL	А	229	57.619	15.419	18.415	1.00	32.34	A
	ATOM	1304	CG2	VAL	Α	229	56.370	16.264	16.436	1.00	34.25	A
	ATOM	1305	С	VAL			57.420	18.035	19.668		37.57	А
50												
50	ATOM	1306	0	VAL	А	229	58.581	18.392	19.474	1.00	35.91	A
	ATOM	1307	N	LEU	Α	230	56.877	17.948	20.878	1.00	40.57	A
							57.615		22.088			
	ATOM	1308	CA	LEU				18.289			46.10	A
	MOTA	1309	СВ	LEU	Α	230	56.654	18.417	23.270	1.00	44.71	A
	ATOM	1310	CG	LEU	Д	230	55.627	19.545	23.207	1.00	44.50	А
55												
55	ATOM	1311		LEU			54.673	19.430	24.383		44.39	A
	MOTA	1312	CD2	LEU	Α	230	56.340	20.885	23.214	1.00	44.81	A
	ATOM	1313	С	LEU	А	230	58.695	17.279	22.440	1.00	50.42	А
	ATOM	1314	0	LEU			58.603	16.104	22.089		51.64	A
	ATOM	1315	N	SER	Α	231	59.717	17.756	23.145	1.00	55.81	A

	ATOM	1316	CA	SER	Α	231	60.824	16.914	23.583	1.00	61.14	А
	ATOM	1317	СВ			231	62.077	17.200	22.750		61.27	А
	ATOM	1318	OG			231	62.444	18.568	22.823		62.85	А
	ATOM	1319	С			231	61.124	17.126	25.071		64.65	А
5	ATOM	1320	0			231	61.392	16.164	25.794		65.70	А
	ATOM	1321	N	PRO	A	232	61.081	18.387	25.549	1.00	67.54	А
	ATOM	1322	CD	PRO	Α	232	60.854	19.651	24.823	1.00	68.60	А
	ATOM	1323	CA	PRO	Α	232	61.358	18.655	26.966	1.00	68.74	A
	ATOM	1324	СВ	PRO	Α	232	61.109	20.158	27.086	1.00	68.83	А
10	ATOM	1325	CG	PRO	Α	232	61.505	20.666	25.737	1.00	68.96	А
	ATOM	1326	С	PRO	Α	232	60.460	17.846	27.899	1.00	69.17	A
	ATOM	1327	0	PRO	Α	232	59.335	17.494	27.541	1.00	69.94	А
	ATOM	1328	N	ALA	Α	237	57.424	23.198	27.637	1.00	80.06	A
	ATOM	1329	CA	ALA	Α	237	56.783	23.047	26.335	1.00	79.29	A
15	ATOM	1330	СВ	ALA	Α	237	55.275	22.907	26.512	1.00	78.64	A
	ATOM	1331	С	ALA	Α	237	57.092	24.239	25.433	1.00	79.07	A
	ATOM	1332	0	ALA	Α	237	56.250	25.113	25.249	1.00	79.47	A
	ATOM	1333	N	ALA	Α	238	58.297	24.280	24.871	1.00	78.57	A
	ATOM	1334	CA	ALA	Α	238	58.683	25.383	23.992	1.00	78.50	A
20	ATOM	1335	СВ	ALA	Α	238	60.186	25.347	23.728	1.00	78.50	A
	ATOM	1336	С	ALA	Α	238	57.920	25.327	22.673	1.00	78.15	A
	ATOM	1337	0	ALA			57.243	24.341	22.375	1.00	77.96	A
	ATOM	1338	N	ALA	Α	239	58.027	26.393	21.887	1.00	77.28	A
	ATOM	1339	CA	ALA			57.338	26.452	20.603		76.27	A
25	ATOM	1340	СВ	ALA			55.849	26.489	20.827		76.61	A
	ATOM	1341	С	ALA			57.766	27.667	19.793		75.38	A
	ATOM	1342	0	ALA			58.955	27.955	19.700		75.89	A
	ATOM	1343	N	ASN			56.781	28.357	19.214		73.95	A
	ATOM	1344	CA	ASN			56.967	29.553	18.389		71.07	A
30	ATOM	1345	СВ	ASN			58.151	30.400	18.874		71.47	A
	ATOM	1346	CG .	ASN			59.459	30.055	18.174		72.06	A
	ATOM	1347		ASN			59.575	30.149	16.943		72.03	A
	ATOM	1348		ASN			60.470	29.665	18.964		71.91	A
2.5	ATOM	1349	С	ASN			57.188	29.178	16.928		69.41	A
35	ATOM	1350	0	ASN			57.480	28.024	16.624		70.09	A
	ATOM	1351	N			241	57.055	30.165	16.038		66.62	A
	ATOM	1352	CA	ALA			57.246	30.013	14.585		63.94	A
	ATOM	1353	C	ALA			55.952	30.080	13.772		60.63	A
40	MOTA	1354 1355	O	ALA			55.840	30.880	12.845		61.29	A
40	MOTA	1356	CB	ALA PHE			57.979 54.984	28.704	14.246		65.23 56.72	A
	ATOM	1356	N CA			242	53.712	29.236 29.196	14.113 13.394		52.53	A
	ATOM ATOM	1357		PHE			53.419	27.767	12.923		49.14	A
	ATOM	1359	CB CG	PHE			52.040	27.590	12.354		47.38	A A
45	ATOM	1360		PHE			51.731	28.067	11.085		47.69	A
73	ATOM	1361		PHE			51.731	26.975	13.102		45.45	A
	ATOM	1362		PHE			50.445	27.937	10.565		46.75	A
	ATOM	1363		PHE			49.751	26.840	12.594		45.41	A
	ATOM	1364	CZ	PHE			49.453	27.323	11.322		46.55	A
50	ATOM	1365	C	PHE			52.534	29.688	14.229		50.08	A
50	ATOM	1366	0	PHE			52.502	29.505	15.444		49.86	A
	ATOM	1367	N	VAL			51.566	30.305	13.557		47.67	A
	ATOM	1368	CA	VAL			50.355	30.809	14.200		46.21	A
	ATOM	1369	CB	VAL			50.340	32.352	14.258		47.36	A
55	ATOM	1370		VAL			49.012	32.844	14.825		47.54	A
-	ATOM	1371		VAL			51.497	32.842	15.109		48.50	A
	ATOM	1372	C	VAL			49.150	30.342	13.389		44.12	A
	ATOM	1373	0	VAL			48.956	30.765	12.247		44.46	A
	ATOM	1374	N	GLY			48.348	29.467	13.985		40.48	А

	ATOM	1375	ca	GLY	Α	244	47.176	28.941	13.306	1.00	37.65	A
	ATOM	1376	С	GLY	Α	244	46.101	29.960	12.964	1.00	35.39	Α
	ATOM	1377	0	GLY			46.313	31.168	13.065		35.92	A
	ATOM	1378	N	THR			44.936	29.463	12.560		33.30	A
5	ATOM	1379	CA	THR	Α	245	43.813	30.312	12.184	1.00	30.20	Α
	ATOM	1380	СВ	THR	Α	245	42.593	29.450	11.829	1.00	32.00	A
	ATOM	1381		THR			42.952	28.573	10.755	1 00	32.81	А
	ATOM	1382		THR			41.419	30.319	11.390		28.34	A
	ATOM	1383	С	THR			43.476	31.296	13.296		27.96	А
10	MOTA	1384	0	THR	Α	245	43.212	30.907	14.434	1.00	25.46	Α
	ATOM	1385	N	ALA	Α	246	43.486	32.576	12.938	1.00	25.22	Α
	ATOM	1386	CA	ALA			43.247	33.675	13.867		23.27	А
	ATOM	1387	СВ	ALA			42.956	34.955	13.082		22.94	A
	ATOM	1388	С	ALA			42.178	33.475	14.934		21.27	А
15	MOTA	1389	0	ALA	Α	246	42.431	33.705	16.114	1.00	20.93	Α
	MOTA	1390	N	GLN	Α	247	40.988	33.047	14.536	1.00	19.67	Α
	ATOM	1391	CA	GLN	Ά	247	39.911	32.886	15.504	1.00	20.17	А
	ATOM	1392	СВ	GLN			38.608	32.535	14.779		21.89	A
	ATOM	1393	CG	GLN			38.522	33.076	13.355		26.18	А
20	ATOM	1394	CD	GLN	Α	247	37.220	33.794	13.064	1.00	27.30	А
	ATOM	1395	OE1	GLN	Α	247	36.172	33.447	13.605	1.00	30.13	A
	ATOM	1396	NE2	GLN	Α	247	37.278	34.792	12.189	1.00	28.70	Α
	ATOM	1397	С	GLN			40.181	31.849	16.595		19.43	А
	ATOM	1398	0	GLN			39.546	31.883	17.648		18.93	А
25	ATOM	1399	N	TYR	Α	248	41.132	30.948	16.359		18.60	А
	MOTA	1400	CA	TYR	Α	248	41.441	29.896	17.329	1.00	19.20	Α
	ATOM	1401	СВ	TYR	Α	248	41.333	28.529	16.642	1.00	17.53	Α
	ATOM	1402	CG	TYR			40.013	28.362	15.927		19.32	А
		1403		TYR			38.859	28.010	16.625		17.69	
30	ATOM											A
30	ATOM	1404		TYR			37.617	27.976	15.990		18.18	A
	MOTA	1405	CD2	TYR	Α	248	39.897	28.664	14.569	1.00	16.87	A
	ATOM	1406	CE2	TYR	Α	248	38.665	28.635	13.924	1.00	19.17	A
	ATOM	1407	CZ	TYR	Α	248	37.527	28.295	14.643	1.00	19.46	A
	ATOM	1408	OH	TYR			36.299	28.311	14.023		18.98	A
35		1409	C	TYR			42.810		17.993		20.42	
33	ATOM							30.039				A
	ATOM	1410	0	TYR			43.208	29.191	18.792		19.19	A
	MOTA	1411	N	VAL	Α	249	43.523	31.114	17.673	1.00	20.20	Α
	MOTA	1412	CA	VAL	Α	249	44.841	31.343	18.251	1.00	20.91	A
	ATOM	1413	СВ	VAL	Α	249	45.542	32.532	17.570		21.18	А
40	ATOM	1414		VAL			46.821	32.896	18.317		22.45	A
70												
	ATOM	1415		VAL			45.862	32.170	16.139		24.01	A
	ATOM	1416	С	VAL			44.764	31.606	19.750		21.52	A
	MOTA	1417	0	VAL	Α	249	43.915	32.368	20.216	1.00	22.72	Α
	MOTA	1418	N	SER	Α	250	45.654	30.965	20.503	1.00	20.70	A
45	ATOM	1419	CA	SER			45.697	31.133	21.951	1.00	21.65	А
	ATOM	1420	СВ	SER			46.370	29.919	22.613		22.02	A
	ATOM	1421	OG	SER			47.692	29.725	22.132		22.12	А
	ATOM	1422	С	SER	Α	250	46.476	32.402	22.280	1.00	22.13	Α
	MOTA	1423	0	SER	Α	250	47.332	32.828	21.511	1.00	22.77	Α
50	ATOM	1424	N	PRO	Α	251	46.180	33.029	23.425		22.23	А
	ATOM	1425	CD	PRO			45.163	32.684	24.433		22.97	A
	ATOM	1426	CA	PRO			46.893	34.254	23.800		22.52	A
	ATOM	1427	СВ	PRO			46.233	34.650	25.127		23.06	Α
	ATOM	1428	CG	PRO	Α	251	45.726	33.329	25.676	1.00	22.55	Α
55	ATOM	1429	С	PRO	Α	251	48.414	34.115	23.907	1.00	22.15	А
	ATOM	1430	0	PRO			49.143	35.047	23.563		22.62	А
	ATOM	1431		GLU			48.901	32.966	24.367		20.69	A
			N									
	ATOM	1432	CA	GLU			50.347	32.772	24.500		21.40	A
	ATOM	1433	СВ	GLU	Α	252	50.673	31.382	25.071	1.00	20.59	А

	ATOM	1434	CG	GLU	Α	252	49.993	30.232	24.352	1.00	21.91	A
	ATOM	1435	CD	GLU	Δ.	252	48.691	29.822	25.014	1 00	21.51	А
	ATOM	1436		GLU			47.989	30.707	25.550		21.46	A
	ATOM	1437	OE2	GLU	Α	252	48.367	28.613	24.993	1.00	20.23	A
5	ATOM	1438	С	GLU	Δ	252	51.071	32.970	23.167	1 00	22.99	A
,												
	MOTA	1439	0	GLU			52.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU	Α	253	50.441	32.576	22.064	1.00	23.00	A
	ATOM	1441	CA	LEU	Α	253	51.068	32.753	20.758	1.00	25.62	A
	ATOM	1442	СВ	LEU			50.277	32.029	19.669		26.75	A
1.0												
10	ATOM	1443	CG	LEU			50.743	30.620	19.296	1.00	31.87	A
	ATOM	1444	CD1	LEU	Α	253	50.433	29.651	20.422	1.00	31.81	A
	ATOM	1445	CD2	LEU	Α	253	50.044	30.179	18.015	1.00	31.86	А
		1446	C	LEU							26.94	
	MOTA						51.201	34.228	20.371			A
	ATOM	1447	0	LEU	Α	253	52.107	34.601	19.626	1.00	27.09	A
15	ATOM	1448	N	LEU	Α	254	50.297	35.059	20.877	1.00	25.83	A
	ATOM	1449	CA	LEU			50.297	36.485	20.564		27.26	А
	MOTA	1450	СВ	LEU			48.858	37.006	20.564		25.84	А
	ATOM	1451	CG	LEU	Α	254	47.882	36.290	19.621	1.00	24.69	A
	ATOM	1452	CD1	LEU	Α	254	46.459	36.724	19.932	1.00	23.64	A
20	ATOM	1453	CD2	LEU	7	254	48.236	36.597	18.177	1 00	24.24	А
20												
	MOTA	1454	С	LEU			51.134	37.314	21.537		30.62	A
	ATOM	1455	0	LEU	Α	254	51.633	38.383	21.187	1.00	32.35	A
	ATOM	1456	N	THR	Α	255	51.292	36.821	22.758	1.00	32.47	А
	ATOM	1457	CA	THR			52.056	37.547	23.759		36.70	A
2.5												
25	ATOM	1458	СВ	THR			51.368	37.478	25.127		34.51	A
	ATOM	1459	OG1	THR	Α	255	51.188	36.106	25.494	1.00	35.49	A
	ATOM	1460	CG2	THR	Α	255	50.013	38.166	25.077	1.00	33.40	А
				THR								
	MOTA	1461	С				53.477	37.035	23.910		40.09	A
	ATOM	1462	0	THR	Α	255	54.430	37.793	23.772	1.00	43.69	A
30	ATOM	1463	N	GLU	Α	256	53.617	35.747	24.189	1.00	44.77	A
	ATOM	1464	CA	GLU	Δ	256	54.932	35.144	24.382	1 00	49.15	A
	MOTA	1465	СВ	GLU			54.866	34.143	25.534		51.24	A
	ATOM	1466	CG	GLU	Α	256	54.514	34.786	26.862	1.00	56.03	A
	ATOM	1467	CD	GLU	Α	256	54.053	33.780	27.893	1.00	58.83	A
35	ATOM	1468		GLU			54.766	32.776	28.107		62.13	А
33												
	MOTA	1469	OE2	GLU			52.979	33.996	28.494		60.34	A
	ATOM	1470	С	GLU	Α	256	55.475	34.456	23.137	1.00	50.09	A
	ATOM	1471	0	GLU	Α	256	56.616	33.995	23.127	1.00	50.42	A
	ATOM	1472	N	LYS			54.658	34.389	22.090		51.21	A
40												
40	ATOM	1473	CA	LYS			55.064	33.746	20.845		51.22	A
	ATOM	1474	CB	LYS	Α	257	56.244	34.502	20.227	1.00	53.28	A
	ATOM	1475	CG	LYS	Α	257	56.558	34.125	18.790	1.00	55.19	A
	ATOM	1476		LYS			57.709	34.961	18.253		57.52	
			CD									A
	MOTA	1477	CE	LYS			57.952	34.694	16.777		58.52	А
45	ATOM	1478	NZ	LYS	Α	257	58.290	33.268	16.515	1.00	60.88	A
	ATOM	1479	С	LYS	Α	257	55.467	32.302	21.138	1.00	50.74	А
	ATOM	1480	0	LYS			56.432	31.790	20.577		52.26	A
	ATOM	1481	N	SER	Α	258	54.721	31.654	22.027	1.00	48.07	A
	ATOM	1482	CA	SER	Α	258	54.999	30.273	22.402	1.00	46.87	A
50	ATOM	1483	СВ	SER			55.590	30.229	23.812	1 00	48.88	А
50												
	ATOM	1484	OG	SER			54.741	30.892	24.734		53.14	A
	ATOM	1485	С	SER	Α	258	53.735	29.415	22.342	1.00	44.07	A
	ATOM	1486	0	SER	Α	258	52.617	29.932	22.417	1.00	44.17	A
	ATOM	1487	N	ALA			53.917	28.105	22.204		38.30	A
55												
55	MOTA	1488	CA	ALA			52.793	27.180	22.127		34.73	A
	ATOM	1489	СВ	ALA			52.551	26.779	20.684	1.00	34.16	A
	MOTA	1490	С	ALA	Α	259	53.042	25.940	22.977	1.00	32.34	A
	ATOM	1491	0	ALA			54.172	25.459	23.086		31.81	A
	MOTA	1492	N	CYS	А	∠60	51.975	25.428	23.579	T.00	28.58	А

	ATOM	1493	CA	CYS	А	260	52.056	24.244	24.425	1.00 26	.27	Α
	ATOM	1494	СВ			260	52.183	24.654	25.892	1.00 26	.53	Α
	ATOM	1495	SG			260	50.846	25.739	26.469	1.00 32		A
	ATOM	1496	C	CYS			50.786	23.435	24.224	1.00 22		A
5	ATOM	1497	0	CYS			49.892	23.856	23.495	1.00 22		A
	ATOM	1498	N	LYS			50.706	22.277	24.868	1.00 20		A
	ATOM	1499	CA	LYS			49.526	21.434	24.744	1.00 20		A
	ATOM	1500	CB	LYS			49.619	20.243	25.696	1.00 23		A
	ATOM	1501	CG			261	50.716	19.253	25.347	1.00 27		A
10	ATOM	1502	CD			261	50.732	18.117	26.350	1.00 27		A
10	ATOM	1502	CE	LYS			51.922	17.203	26.134	1.00 23		A
	ATOM	1504	ΝZ	LYS			51.940	16.121	27.153	1.00 32		A
	ATOM	1505	C	LYS			48.268	22.229	25.062	1.00 19		A
	ATOM	1506	0	LYS			47.253	22.092	24.387	1.00 19		A
15		1507		SER			47.253	23.068	24.307	1.00 16		
13	ATOM	1507	N	SER			47.235	23.883	26.534	1.00 18		A
	ATOM		CA									A
	ATOM	1509	CB	SER			47.644	24.698	27.770	1.00 18		A
	ATOM	1510	OG G			262	46.517	25.258	28.421	1.00 22		A
20	ATOM	1511	C			262	46.736	24.811	25.424	1.00 16		A
20	ATOM	1512	0	SER			45.591	25.254	25.450	1.00 15		A
	ATOM	1513	N	SER			47.595	25.118	24.456	1.00 16		A
	ATOM	1514	CA	SER			47.175	25.970	23.347	1.00 16		A
	ATOM	1515	СВ			263	48.340	26.228	22.382	1.00 18		A
25	ATOM	1516	OG G			263	49.402	26.909	23.031 22.612	1.00 22 1.00 17		A
23	ATOM	1517 1518	C			263	46.040 45.099	25.257 25.898	22.612	1.00 17		A
	ATOM		O			263						A
	ATOM	1519 1520	N	ASP			46.119	23.928	22.517	1.00 16		A
	ATOM		CA	ASP			45.069	23.166	21.836	1.00 16		A
30	ATOM	1521 1522	CB CG	ASP			45.483 46.544	21.704 21.539	21.620 20.548	1.00 15 1.00 17		A A
30	ATOM ATOM	1523		ASP ASP			46.544	22.412	19.661	1.00 17		A
	ATOM	1524		ASP			47.265	20.515	20.579	1.00 16		A
	ATOM	1525	C C	ASP			43.773	23.194	22.646	1.00 10		A
	ATOM	1526	0	ASP			42.681	23.194	22.046	1.00 17		A
35	ATOM	1527	N	LEU			43.898	23.205	23.974	1.00 15		A
33	ATOM	1527	CA	LEU			42.730	23.232	24.849	1.00 13		A
		1529				265		23.232	26.313	1.00 14		
	ATOM	1530	CB	LEU			43.147			1.00 11		A
	ATOM	1530	CG				43.711	21.641	26.621 28.052	1.00 14		A
40	MOTA	1531		LEU LEU			44.249 42.619	21.579 20.603	26.416	1.00 13		A A
40	ATOM	1532	CDZ	LEU				24.557	24.675	1.00 11		
	MOTA	1534	0	LEU			41.999 40.777	24.620	24.873	1.00 15		A
	ATOM ATOM	1535	N	TRP			42.746	25.622	24.705	1.00 16		A
	ATOM	1536	CA			266	42.748	26.918	24.403	1.00 16		A A
45	ATOM	1537	CB			266	43.176	28.015	24.104	1.00 10		A
43			СБ			266	42.618			1.00 17		
	ATOM	1538 1539		TRP			42.313	29.326 30.490	23.521 24.301	1.00 20		A A
	ATOM ATOM	1540		TRP			41.782	31.459	23.417	1.00 20		A
	ATOM	1541		TRP			42.435	30.810	25.660	1.00 20		A
50	ATOM	1541		TRP			42.433	29.631	22.231	1.00 20		A
50	ATOM	1543		TRP			41.769	30.908	22.163	1.00 19		A
	ATOM	1544		TRP			41.372	32.727	23.850	1.00 20		A
	ATOM	1545		TRP			42.026	32.727	26.091	1.00 20		A
	ATOM	1546		TRP			41.501	33.015	25.185	1.00 20		A
55	ATOM	1547	C	TRP			41.284	26.795	22.913	1.00 20		A
22	ATOM	1548	0	TRP			40.139	27.240	22.863	1.00 17		A
	ATOM	1549	N	ALA			41.863	26.181	21.886	1.00 17		A
	ATOM	1550	CA	ALA			41.155	25.990	20.626	1.00 17		A
	ATOM	1551	CB	ALA			42.050	25.290	19.621	1.00 10		A
	111 011	1001	010	4 2414 1	2.1	,	12.000		· · · ·	UU 17		4 1

	ATOM	1552	С	ALA	Α	267	39.901	25.159	20.891	1.00 16.3	28 A
	ATOM	1553	0	ALA			38.835	25.436	20.346	1.00 16.	
	ATOM	1554	N			268	40.031	24.144	21.739	1.00 16.	
	ATOM	1555	CA	LEU	Α	268	38.890	23.299	22.084	1.00 17.	
5	ATOM	1556	СВ			268	39.292	22.260	23.139	1.00 15.	
	ATOM	1557	CG	LEU	Α	268	38.158	21.429	23.754	1.00 19.	
	ATOM	1558	CD1	LEU	Α	268	37.505	20.578	22.678	1.00 16.	
	ATOM	1559	CD2	LEU	Α	268	38.718	20.537	24.881	1.00 17.	49 A
	ATOM	1560	С	LEU	А	268	37.766	24.179	22.628	1.00 15.	72 A
10	ATOM	1561	0	LEU	Α	268	36.603	24.031	22.247	1.00 15.	28 A
	ATOM	1562	N	GLY	Α	269	38.119	25.099	23.520	1.00 14.	34 A
	ATOM	1563	CA	GLY	Α	269	37.124	25.989	24.092	1.00 13.	39 A
	ATOM	1564	С	GLY	Α	269	36.406	26.808	23.031	1.00 14.	94 A
	MOTA	1565	0	GLY	Α	269	35.193	27.014	23.114	1.00 14.	76 A
15	MOTA	1566	N	CYS	Α	270	37.146	27.279	22.030	1.00 13.	36 A
	MOTA	1567	CA	CYS	Α	270	36.539	28.061	20.958	1.00 16.	80 A
	MOTA	1568	СВ	CYS	Α	270	37.611	28.634	20.023	1.00 15.	97 A
	MOTA	1569	SG	CYS	Α	270	38.751	29.810	20.780	1.00 20.	48 A
	ATOM	1570	С	CYS	Α	270	35.598	27.175	20.140	1.00 17.	50 A
20	ATOM	1571	0	CYS	Α	270	34.516	27.604	19.741	1.00 18.	38 A
	ATOM	1572	N	ILE	Α	271	36.022	25.939	19.887	1.00 16.	99 A
	ATOM	1573	CA	ILE	Α	271	35.221	25.004	19.104	1.00 16.	66 A
	ATOM	1574	СВ	ILE	Α	271	36.038	23.741	18.778	1.00 16.	53 A
	ATOM	1575	CG2	ILE	Α	271	35.155	22.694	18.102	1.00 16.	34 A
25	MOTA	1576	CG1	ILE	Α	271	37.222	24.129	17.882	1.00 15.	59 A
	MOTA	1577	CD1	ILE	Α	271	38.239	23.018	17.690	1.00 14.	88 A
	MOTA	1578	С	ILE	Α	271	33.920	24.626	19.809	1.00 16.	74 A
	ATOM	1579	0			271	32.865	24.576	19.179	1.00 17.	
	ATOM	1580	N			272	33.990	24.357	21.111	1.00 16.	
30	ATOM	1581	CA			272	32.785	24.021	21.862	1.00 18.	
	ATOM	1582	СВ			272	33.097	23.747	23.346	1.00 17.	
	ATOM	1583	CG2				31.796	23.666	24.152	1.00 17.	
	ATOM	1584	CG1				33.877	22.437	23.481	1.00 19.	
	MOTA	1585		ILE			34.446	22.217	24.886	1.00 18.	
35	MOTA	1586	С			272	31.824	25.207	21.776	1.00 19.	
	MOTA	1587	0			272	30.624	25.037	21.554	1.00 20.	
	MOTA	1588	N			273	32.362	26.409	21.947	1.00 18.	
	ATOM	1589	CA			273	31.553	27.615	21.881	1.00 20.	
40	ATOM	1590	СВ			273	32.418	28.847	22.162	1.00 18.	
40	ATOM	1591	CG			273	31.663	30.161	22.125	1.00 20.	
	ATOM	1592	CD1				31.229	30.709	20.916	1.00 20.	
	ATOM	1593	CE1				30.536	31.917	20.880	1.00 20.	
	ATOM	1594		TYR			31.383	30.857	23.302	1.00 19.	
4.5	ATOM	1595		TYR			30.691	32.062	23.280	1.00 20.	
45	ATOM	1596	CZ			273	30.271	32.587	22.067	1.00 21.	
	ATOM	1597	OH			273	29.588	33.776	22.049	1.00 21.	
	ATOM	1598	C			273	30.902	27.730	20.507	1.00 21.	
	ATOM	1599	0			273	29.719	28.049	20.401	1.00 22.	
50	ATOM	1600	N			274	31.676	27.454	19.461		
50	ATOM	1601 1602	CA CB			274	31.176	27.538 27.341	18.095 17.097	1.00 21.	
	ATOM		СБ	GLN		274	32.323	27.596		1.00 21.	
	ATOM	1603 1604	CD				31.934	27.588	15.645 14.706	1.00 23.	
	ATOM ATOM	1604		GLN		274 274	33.131 34.276	27.300	15.139	1.00 24.	
55		1605		GLN				27.446	13.139	1.00 22.	
55	ATOM ATOM	1607	NEZ C			274	32.870 30.076	26.517	17.828	1.00 22.	
	ATOM	1607	0	GLN			29.123	26.806	17.108	1.00 21.	
	ATOM	1609	N			275	30.207	25.324	18.403	1.00 20.	
	ATOM	1610	CA			275	29.196	24.282	18.208	1.00 21.	
	ATON	TOTO	O.A.	∪نن∟	17	215	△ J • ⊥ J U	47.404	10.200	1.00 20.	A

	ATOM	1611	CB	LEU	Α	275	29.645	22.958	18.846	1.00	19.11	A
	ATOM	1612	CG	LEU	Ζ	275	30.775	22.182	18.159	1.00	21 43	А
	ATOM	1613		LEU			31.118	20.936	18.963	1.00		Α
	ATOM	1614	CD2	LEU	Α	275	30.342	21.795	16.754	1.00	20.34	Α
5	ATOM	1615	С	LEU	Δ	275	27.860	24.697	18.815	1.00	21 32	А
,												
	ATOM	1616	0	LEU			26.802	24.461	18.229	1.00		А
	ATOM	1617	N	VAL	Α	276	27.921	25.322	19.987	1.00	19.10	Α
	ATOM	1618	CA	VAL	Α	276	26.724	25.750	20.702	1.00	22.47	Α
	ATOM	1619	СВ	VAL			27.011	25.882	22.217	1.00		A
1.0												
10	ATOM	1620	CGI	VAL	А	276	25.742	26.291	22.957	1.00	19.68	А
	ATOM	1621	CG2	VAL	Α	276	27.550	24.558	22.766	1.00	19.43	Α
	ATOM	1622	С	VAL	Δ	276	26.127	27.075	20.211	1.00	23 89	Α
	ATOM	1623	0	VAL			24.910	27.199	20.070	1.00		А
	ATOM	1624	N	ALA	Α	277	26.983	28.062	19.965	1.00	24.56	Α
15	ATOM	1625	CA	ALA	Α	277	26.533	29.374	19.518	1.00	24.72	Α
	ATOM	1626	СВ	ALA			27.504	30.444	19.999	1.00		A
	ATOM	1627	С	ALA			26.378	29.458	18.005	1.00		Α
	ATOM	1628	0	ALA	Α	277	25.577	30.242	17.502	1.00	26.39	Α
	ATOM	1629	N	GLY	Α	278	27.142	28.651	17.280	1.00	25.13	А
20									15.834			
20	ATOM	1630	CA	GLY			27.062	28.673		1.00		A
	ATOM	1631	С	GLY	Α	278	28.163	29.524	15.231	1.00	26.50	Α
	MOTA	1632	0	GLY	Α	278	28.374	29.510	14.015	1.00	28.17	Α
	ATOM	1633	N	LEU			28.866	30.262	16.086	1.00		А
	ATOM	1634	CA	LEU			29.962	31.130	15.656	1.00		А
25	ATOM	1635	СВ	LEU	Α	279	29.468	32.575	15.500	1.00	25.78	Α
	ATOM	1636	CG	LEU	Α	279	28.364	32.899	14.490	1.00	28.17	A
	ATOM	1637		LEU			27.922	34.344	14.684	1.00		A
	ATOM	1638	CD2	LEU	А	279	28.862	32.670	13.071	1.00	26.52	Α
	ATOM	1639	С	LEU	Α	279	31.093	31.116	16.687	1.00	23.47	Α
30	ATOM	1640	0	LEU	Α	279	30.848	30.994	17.882	1.00	24.44	Α
50							32.349					A
	ATOM	1641	N	PRO				31.239	16.236	1.00		
	ATOM	1642	CD	PRO	Α	280	32.831	31.404	14.855	1.00	22.26	Α
	ATOM	1643	CA	PRO	Α	280	33.464	31.239	17.189	1.00	23.81	Α
	ATOM	1644	СВ	PRO			34.692	31.293	16.282	1.00		A
2.5												
35	ATOM	1645	CG	PRO	А	280	34.189	32.020	15.073	1.00		Α
	ATOM	1646	С	PRO	Α	280	33.353	32.444	18.137	1.00	22.69	\mathbf{A}
	ATOM	1647	0	PRO	Ά	280	32.750	33.457	17.788	1.00	22.11	Α
	ATOM	1648		PRO			33.939	32.344	19.345	1.00		A
			N									
	ATOM	1649	CD	PRO	Α	281	34.810	31.223	19.734	1.00		Α
40	ATOM	1650	CA	PRO	Α	281	33.935	33.375	20.395	1.00	23.67	Α
	ATOM	1651	СВ	PRO	Δ	281	34.781	32.751	21.509	1.00	24 89	А
	ATOM	1652	CG	PRO			34.749	31.287	21.219	1.00		А
	ATOM	1653	С	PRO	Α	281	34.481	34.752	20.017	1.00	23.75	Α
	MOTA	1654	0	PRO	Α	281	33.869	35.781	20.317	1.00	21.02	Α
45	ATOM	1655	N	PHE	Ζ.	282	35.644	34.763	19.379	1.00		А
73												
	ATOM	1656	CA	PHE			36.293	36.007	18.998	1.00		Α
	ATOM	1657	CB	PHE	Α	282	37.765	35.943	19.406	1.00	21.01	\mathbf{A}
	ATOM	1658	CG	PHE	Α	282	37.975	35.482	20.822	1.00	22.66	Α
	ATOM	1659		PHE			37.806	36.361	21.888	1.00		A
50												
50	ATOM	1660		PHE			38.291	34.151	21.093	1.00		А
	ATOM	1661	CE1	PHE	Α	282	37.947	35.921	23.206	1.00	22.66	Α
	ATOM	1662		PHE			38.433	33.702	22.405	1.00		А
	ATOM	1663	CZ	PHE			38.261	34.590	23.466	1.00		A
	MOTA	1664	С	PHE	Α	282	36.169	36.263	17.503	1.00	24.39	Α
55	MOTA	1665	0	PHE	Α	282	36.802	35.585	16.694	1.00	25.80	Α
	ATOM	1666	N	ARG			35.355	37.248	17.142	1.00		A
	ATOM	1667	CA	ARG			35.141	37.594	15.741	1.00		А
	MOTA	1668	СВ	ARG	Α	283	33.721	37.209	15.316	1.00	28.91	Α
	ATOM	1669	CG	ARG	А	283	33.293	35.808	15.724	1.00	30.27	А

	MOTA	1670	CD	ARG	Α	283	31.904	35.493	15.188	1.00	33.36	A
	ATOM	1671	NE	ARG	Α	283	30.890	36.392	15.733	1.00	32.76	А
	ATOM	1672	CZ	ARG			30.372	36.287	16.952		34.79	A
	MOTA	1673		ARG			30.767	35.317	17.768		35.77	A
5	ATOM	1674	NH2	ARG	Α	283	29.458	37.156	17.359	1.00	36.12	A
	ATOM	1675	С	ARG	Α	283	35.328	39.096	15.544	1.00	26.47	А
	ATOM	1676	0	ARG			35.029	39.888	16.438	1 00	26.28	А
							35.818				26.70	
	ATOM	1677	N	ALA				39.486	14.373			A
	MOTA	1678	CA	ALA			36.033	40.899	14.079		27.84	A
10	ATOM	1679	СВ	ALA	Α	284	37.188	41.442	14.914	1.00	26.24	A
	ATOM	1680	С	ALA	Α	284	36.327	41.077	12.602	1.00	28.35	A
	ATOM	1681	0	ALA	Α	284	36.560	40.101	11.891	1.00	29.91	А
	ATOM	1682	N			285	36.332	42.329	12.153		29.29	A
1.7	ATOM	1683	CA	GLY			36.577	42.631	10.753		29.52	A
15	ATOM	1684	С	GLY	А	285	37.893	42.156	10.168		30.12	А
	ATOM	1685	0	$\operatorname{GL} Y$	Α	285	37.974	41.862	8.976	1.00	30.60	A
	ATOM	1686	N	ASN	Α	286	38.939	42.097	10.983	1.00	28.49	A
	ATOM	1687	CA	ASN	Δ	286	40.231	41.644	10.489	1.00	26.71	А
	ATOM	1688	CB	ASN			41.050	42.825	9.945		26.11	A
20												
20	ATOM	1689	CG	ASN			41.310	43.900	10.990		27.83	A
	ATOM	1690		ASN			41.877	43.631	12.049	1.00	27.84	A
	ATOM	1691	ND2	ASN	Α	286	40.908	45.131	10.685	1.00	25.95	A
	ATOM	1692	С	ASN	Α	286	40.997	40.924	11.584	1.00	26.03	А
	ATOM	1693	0	ASN			40.540	40.851	12.723		25.66	А
25		1694		GLU				40.391			24.81	
23	ATOM		N				42.162		11.239			A
	MOTA	1695	CA			287	42.965	39.662	12.206		27.59	A
	ATOM	1696	СВ	GLU	Α	287	44.145	38.985	11.510	1.00	30.17	A
	ATOM	1697	CG	GLU	Α	287	43.776	37.632	10.931	1.00	38.21	A
	ATOM	1698	CD	GLU	Α	287	44.900	36.998	10.140	1.00	41.86	А
30	ATOM	1699		GLU			46.061	37.036	10.608		43.08	A
30		1700		GLU					9.052			A
	ATOM						44.612	36.449			45.22	
	ATOM	1701	С	GLU			43.459	40.485	13.383		25.05	A
	ATOM	1702	0	GLU	Α	287	43.382	40.030	14.521		26.41	A
	ATOM	1703	N	TYR	Α	288	43.966	41.685	13.122	1.00	23.04	A
35	ATOM	1704	CA	TYR	Α	288	44.460	42.528	14.205		22.34	А
	ATOM	1705	СВ	TYR			44.867	43.913	13.691		21.07	A
	ATOM	1706	CG	TYR			45.275	44.858	14.805		21.07	A
	MOTA	1707		TYR			46.533	44.762	15.405		21.23	A
	ATOM	1708	CE1	TYR	Α	288	46.891	45.588	16.475	1.00	20.43	A
40	ATOM	1709	CD2	TYR	Α	288	44.380	45.809	15.302	1.00	22.32	A
	ATOM	1710	CE2	TYR	Α	288	44.725	46.637	16.373	1.00	23.28	А
	ATOM	1711	CZ	TYR			45.981	46.518	16.953		22.96	A
	ATOM	1712	OH	TYR			46.316	47.313	18.024		23.18	A
	MOTA	1713	С	TYR			43.402	42.698	15.288		21.38	A
45	ATOM	1714	0	TYR	Α	288	43.710	42.616	16.473	1.00	22.09	A
	ATOM	1715	N	LEU	Α	289	42.159	42.939	14.874	1.00	21.88	A
	ATOM	1716	CA	LEU	Δ	289	41.055	43.130	15.811		21.98	A
	ATOM	1717	СВ	LEU			39.821	43.673	15.078		22.90	A
	MOTA	1718	CG	LEU			39.896	45.130	14.601		26.52	A
50	MOTA	1719	CD1	LEU	А	289	38.706	45.436	13.696	1.00	26.55	A
	ATOM	1720	CD2	LEU	Α	289	39.914	46.071	15.807	1.00	23.13	A
	ATOM	1721	С	LEU	Α	289	40.686	41.849	16.560		21.24	А
	ATOM	1722	0	LEU			40.256	41.897	17.715		20.72	A
								40.708				
	ATOM	1723	N	ILE			40.843		15.900		19.62	A
55	MOTA	1724	CA			290	40.538	39.433	16.533		18.54	A
	ATOM	1725	СВ	ILE	Α	290	40.560	38.281	15.509	1.00	18.52	A
	MOTA	1726	CG2	ILE	Α	290	40.503	36.934	16.234	1.00	17.63	A
	ATOM	1727		ILE			39.378	38.429	14.545	1.00	18.88	A
	ATOM	1728		ILE			39.421	37.483	13.357		19.81	A
	VI OIJ	1/40	CDT	ظست	ч	200	J J • 441	J/. TUJ	±0.001	T.00	T).0T	A

	ATOM	1729	С	ILE	A	290	41.578	39.167	17.618	1.00	19.09	A
	ATOM	1730	0	ILE	Α	290	41.236	38.788	18.737	1.00	18.20	A
	ATOM	1731	N	PHE	Α	291	42.849	39.376	17.286	1.00	18.76	A
	ATOM	1732	CA	PHE	А	291	43.925	39.156	18.247	1.00	20.75	A
5	ATOM	1733	СВ	PHE	Α	291	45.286	39.434	17.606	1.00	20.71	A
	ATOM	1734	CG	PHE	Α	291	45.644	38.480	16.503	1.00	22.92	A
	ATOM	1735	CD1	PHE	Α	291	45.065	37.214	16.443	1.00	22.98	A
	ATOM	1736	CD2	PHE	Α	291	46.588	38.830	15.543	1.00	22.91	A
	ATOM	1737	CE1	PHE	Α	291	45.423	36.310	15.440	1.00	24.51	A
10	ATOM	1738	CE2	PHE	Α	291	46.954	37.931	14.535	1.00	25.54	A
	ATOM	1739	CZ	PHE	Α	291	46.370	36.670	14.485	1.00	23.29	A
	ATOM	1740	С	PHE	Α	291	43.739	40.061	19.451	1.00	21.72	A
	ATOM	1741	0	PHE	Α	291	43.992	39.671	20.593	1.00	22.32	A
	ATOM	1742	N	GLN	Α	292	43.284	41.275	19.178	1.00	23.27	A
15	ATOM	1743	CA	GLN	Α	292	43.055	42.264	20.216	1.00	24.01	A
	ATOM	1744	СВ	GLN	Α	292	42.574	43.559	19.562	1.00	25.77	A
	ATOM	1745	CG	GLN	Α	292	42.577	44.773	20.447	1.00	28.45	A
	ATOM	1746	CD	GLN	Α	292	42.469	46.057	19.638	1.00	29.83	A
	ATOM	1747	OE1	GLN	Α	292	41.520	46.244	18.872	1.00	27.16	A
20	ATOM	1748	NE2	GLN	Α	292	43.449	46.944	19.799	1.00	27.61	A
	ATOM	1749	С	GLN	Α	292	42.018	41.733	21.204	1.00	22.97	A
	ATOM	1750	0	GLN	Α	292	42.200	41.832	22.415	1.00	21.64	A
	ATOM	1751	N	LYS	Α	293	40.937	41.154	20.687	1.00	21.82	A
	ATOM	1752	CA	LYS	Α	293	39.895	40.612	21.558	1.00	22.18	A
25	ATOM	1753	СВ	LYS	Α	293	38.664	40.223	20.740	1.00	22.69	A
	ATOM	1754	CG	LYS	Α	293	37.919	41.407	20.153	1.00	25.78	A
	ATOM	1755	CD	LYS	Α	293	36.651	40.961	19.429	1.00	27.88	A
	ATOM	1756	CE	LYS	Α	293	35.857	42.161	18.926	1.00	30.85	A
	ATOM	1757	NZ	LYS	Α	293	34.612	41.750	18.214	1.00	32.98	А
30	ATOM	1758	С	LYS	Α	293	40.398	39.398	22.343	1.00	21.20	A
	ATOM	1759	0	LYS	Α	293	40.041	39.204	23.509	1.00	22.01	А
	ATOM	1760	N	ILE	Α	294	41.226	38.583	21.702	1.00	19.91	А
	ATOM	1761	CA	ILE			41.774	37.394	22.347		20.28	А
	ATOM	1762	СВ	ILE			42.631	36.575	21.349		18.98	А
35	ATOM	1763	CG2	ILE	Α	294	43.481	35.550	22.098	1.00	17.70	А
	ATOM	1764	CG1	ILE			41.716	35.897	20.318		17.93	А
	ATOM	1765	CD1	ILE	Α	294	42.467	35.237	19.178	1.00	16.21	А
	ATOM	1766	С	ILE	Α	294	42.618	37.727	23.587		21.94	А
	ATOM	1767	0	ILE	Α	294	42.366	37.199	24.673	1.00	20.86	А
40	ATOM	1768	N	ILE			43.610	38.600	23.439		21.88	А
	ATOM	1769	CA			295	44.461	38.934	24.582		24.25	А
	ATOM	1770	СВ	ILE	Α	295	45.668	39.805	24.175	1.00	23.93	А
	ATOM	1771	CG2	ILE	Α	295	46.514	39.066	23.140	1.00	24.61	A
	ATOM	1772	CG1	ILE	Α	295	45.189	41.151	23.637		24.58	А
45	ATOM	1773		ILE			46.317	42.149	23.433		26.69	А
	ATOM	1774	С	ILE	Α	295	43.720	39.636	25.717		24.80	А
	ATOM	1775	0			295	44.214	39.687	26.842	1.00	24.76	А
	ATOM	1776	N			296	42.539	40.173	25.425		25.33	А
	ATOM	1777	CA			296	41.743	40.853	26.444		26.80	А
50	ATOM	1778	СВ	LYS			41.178	42.170	25.894	1.00	27.39	А
	ATOM	1779	CG	LYS			42.240	43.141	25.413		31.79	А
	ATOM	1780	CD	LYS			41.634	44.410	24.826		35.56	А
	ATOM	1781	CE	LYS			41.009	45.283	25.900		39.29	А
	ATOM	1782	ΝZ	LYS			40.564	46.603	25.357		41.72	A
55	ATOM	1783	C	LYS			40.593	39.958	26.893		25.50	A
	ATOM	1784	0	LYS			39.770	40.361	27.713		24.02	A
	ATOM	1785	N	LEU			40.550	38.742	26.349		25.67	A
	ATOM	1786	CA	LEU			39.500	37.777	26.666		25.16	A
	ATOM	1787	СВ	LEU			39.632	37.285	28.111		24.80	A
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	ATOM	1788	CG	LEU	Α	297	38.766	36.068	28.460	1.00	26.43	A
	ATOM	1789	CD1	LEU	7	297	39.238	34.852	27.646	1 00	26.70	А
	ATOM	1790	CD2	LEU			38.856	35.777	29.951		24.84	A
	MOTA	1791	С	LEU	Α	297	38.151	38.459	26.467	1.00	25.11	A
5	ATOM	1792	0	LEU	Δ	297	37.261	38.378	27.309	1.00	25.28	A
,											24.98	
	ATOM	1793	N	GLU			38.007	39.127	25.331			A
	MOTA	1794	CA	GLU	Α	298	36.786	39.847	25.023	1.00	25.31	A
	ATOM	1795	СВ	GLU	A	298	37.143	41.139	24.291	1.00	27.13	A
	ATOM	1796	CG	GLU			35.991	42.092	24.108		31.28	A
1.0												
10	MOTA	1797	CD	GLU			36.419	43.362	23.410		34.40	A
	MOTA	1798	OE1	GLU	Α	298	37.348	44.027	23.918	1.00	35.90	A
	ATOM	1799	OE2	GLU	Α	298	35.832	43.693	22.359	1.00	36.16	А
		1800	C	GLU				39.057			23.79	
	ATOM						35.766		24.207			A
	ATOM	1801	0	GLU	Α	298	35.832	39.017	22.979	1.00	24.35	A
15	ATOM	1802	N	TYR	Α	299	34.825	38.427	24.902	1.00	23.45	A
	ATOM	1803	CA	TYR	Δ	299	33.760	37.663	24.265	1 00	23.98	А
	ATOM	1804	СВ	TYR			34.264	36.304	23.755		20.13	А
	MOTA	1805	CG	TYR	Α	299	34.348	35.233	24.828	1.00	21.17	A
	ATOM	1806	CD1	TYR	Α	299	35.336	35.279	25.810	1.00	19.32	А
20	ATOM	1807		TYR			35.389	34.332	26.826		19.30	A
20												
	ATOM	1808	CD2	TYR	А	299	33.410	34.201	24.888	1.00	18.96	A
	MOTA	1809	CE2	TYR	Α	299	33.456	33.243	25.907	1.00	19.41	A
	ATOM	1810	CZ	TYR	Δ	299	34.449	33.321	26.870	1.00	18.79	А
		1811										
	ATOM		OH	TYR			34.511	32.401	27.881		18.77	А
25	MOTA	1812	С	TYR	Α	299	32.699	37.437	25.331	1.00	25.20	A
	ATOM	1813	0	TYR	Α	299	32.942	37.681	26.506	1.00	26.46	A
	ATOM	1814	N	ASP	Δ	300	31.522	36.981	24.927	1 00	26.94	А
	ATOM	1815	CA	ASP			30.467	36.710	25.891		30.60	A
	ATOM	1816	СВ	ASP	Α	300	29.665	37.981	26.179	1.00	35.86	A
30	ATOM	1817	CG	ASP	Α	300	29.228	38.687	24.923	1.00	42.04	A
	ATOM	1818		ASP			28.450	38.088	24.149		45.98	A
	ATOM	1819	OD2	ASP			29.666	39.840	24.707		45.69	A
	ATOM	1820	С	ASP	Α	300	29.564	35.608	25.363	1.00	29.26	A
	ATOM	1821	0	ASP	Α	300	29.590	35.299	24.172	1.00	28.64	A
35	ATOM	1822	N	PHE			28.778	35.011	26.253		28.96	A
33												
	ATOM	1823	CA	PHE	Α	301	27.884	33.924	25.871	1.00	30.48	A
	ATOM	1824	CB	PHE	Α	301	27.818	32.854	26.968	1.00	29.17	A
	ATOM	1825	CG	PHE	Δ	301	29.147	32.279	27.356	1.00	29.29	A
		1826		PHE			29.978				27.31	
	ATOM							32.949	28.245			A
40	MOTA	1827	CD2	PHE	Α	301	29.560	31.050	26.845	1.00	27.89	A
	ATOM	1828	CE1	PHE	Α	301	31.205	32.403	28.625	1.00	28.83	A
	ATOM	1829	CE2	PHE	Ζ	301	30.781	30.498	27.217	1 00	28.05	А
	ATOM	1830	CZ	PHE			31.605	31.175	28.110		28.27	A
	MOTA	1831	С	PHE	Α	301	26.459	34.384	25.619	1.00	32.20	A
45	ATOM	1832	0	PHE	Α	301	25.946	35.261	26.317	1.00	32.36	A
	ATOM	1833	N	PRO			25.798	33.804	24.607		33.29	А
	ATOM	1834	CD	PRO	Α	302	26.313	32.943	23.529		34.04	A
	ATOM	1835	CA	PRO	Α	302	24.415	34.199	24.341	1.00	35.24	A
	ATOM	1836	СВ	PRO	Α	302	24.144	33.608	22.959	1.00	34.01	A
50	ATOM	1837	CG	PRO			25.041	32.413	22.921		35.48	A
50												
	ATOM	1838	С	PRO	А	302	23.567	33.561	25.444	1.00	37.39	A
	ATOM	1839	0	PRO	Α	302	23.935	32.518	25.986	1.00	38.49	A
	ATOM	1840	N	ALA			22.447	34.188	25.783		39.36	А
	ATOM	1841	CA	ALA			21.572	33.692	26.843		40.65	A
55	ATOM	1842	СВ	ALA			20.280	34.506	26.862		41.66	A
	ATOM	1843	С	ALA	Α	303	21.238	32.197	26.814	1.00	41.25	A
	ATOM	1844	0	ALA			21.253	31.537	27.854		43.16	А
	ATOM	1845	N	ALA			20.945	31.665	25.631		41.04	A
	ATOM	1846	CA	ALA	А	304	20.569	30.258	25.480	1.00	40.66	A

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	ATOM	1847	СВ	ALA	Α	304	20.121	30.004	24.040	1.00 41.36	A
	ATOM	1848	С	ALA	Α	304	21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	0	ALA	Ά	304	21.298	28.156	26.395	1.00 40.61	A
	ATOM	1850	N	PHE			22.891	29.543	25.617	1.00 36.21	A
-											
5	MOTA	1851	CA	PHE			24.022	28.662	25.909	1.00 32.08	A
	ATOM	1852	СВ	PHE	Α	305	25.259	29.519	26.187	1.00 29.46	A
	ATOM	1853	CG	PHE	Α	305	26.536	28.917	25.690	1.00 28.15	A
	ATOM	1854	CD1	PHE	Α	305	27.146	27.875	26.377	1.00 26.20	A
	ATOM	1855		PHE			27.127	29.386	24.521	1.00 27.05	А
10	ATOM	1856		PHE			28.330	27.308	25.908	1.00 26.92	A
10											
	MOTA	1857	CE2	PHE			28.312	28.826	24.042	1.00 26.62	A
	ATOM	1858	CZ	PHE			28.914	27.786	24.737	1.00 26.61	A
	ATOM	1859	С	PHE	Α	305	23.811	27.664	27.057	1.00 30.09	A
	ATOM	1860	0	PHE	Α	305	23.518	28.051	28.187	1.00 31.51	А
15	ATOM	1861	N	PHE			23.964	26.378	26.758	1.00 27.01	А
	ATOM	1862	CA	PHE			23.801	25.334	27.769	1.00 26.30	A
	ATOM	1863	СВ	PHE			24.157	23.970	27.170	1.00 25.03	A
	ATOM	1864	CG	PHE			23.548	23.725	25.815	1.00 27.24	A
	ATOM	1865	CD1	PHE	Α	306	22.170	23.831	25.622	1.00 28.40	A
20	ATOM	1866	CD2	PHE	Α	306	24.350	23.386	24.728	1.00 27.84	A
	ATOM	1867	CE1	PHE	Α	306	21.601	23.603	24.365	1.00 28.05	A
	ATOM	1868		PHE			23.792	23.155	23.465	1.00 28.31	A
	ATOM	1869	CZ	PHE			22.415	23.263	23.283	1.00 28.00	A
	ATOM	1870	С	PHE			24.711	25.652	28.961	1.00 26.23	А
25	ATOM	1871	0	PHE	Α	306	25.927	25.775	28.811	1.00 25.59	A
	MOTA	1872	N	PRO	Α	307	24.125	25.796	30.163	1.00 26.67	A
	ATOM	1873	CD	PRO	Α	307	22.685	25.625	30.430	1.00 27.95	A
	ATOM	1874	CA	PRO			24.842	26.110	31.405	1.00 26.59	A
		1875	СВ	PRO			23.795	25.832	32.481	1.00 26.14	
20	ATOM										A
30	ATOM	1876	CG	PRO			22.531	26.250	31.803	1.00 27.86	A
	ATOM	1877	С	PRO	Α	307	26.145	25.355	31.659	1.00 25.58	A
	ATOM	1878	0	PRO	Α	307	27.189	25.964	31.900	1.00 22.65	A
	ATOM	1879	N	LYS	Α	308	26.085	24.031	31.620	1.00 24.46	A
	ATOM	1880	CA	LYS	Α	308	27.274	23.232	31.867	1.00 23.91	A
35	ATOM	1881	СВ	LYS			26.887	21.760	32.024	1.00 23.25	A
33											
	ATOM	1882	CG	LYS			26.062	21.532	33.285	1.00 28.49	A
	ATOM	1883	CD	LYS			25.618	20.093	33.466	1.00 30.17	A
	MOTA	1884	CE	LYS	Α	308	24.760	19.973	34.722	1.00 33.12	A
	MOTA	1885	NZ	LYS	Α	308	24.122	18.636	34.860	1.00 34.13	A
40	ATOM	1886	С	LYS	Α	308	28.314	23.426	30.769	1.00 22.84	A
	ATOM	1887	0	LYS			29.514	23.411	31.042	1.00 22.46	A
	ATOM	1888	N	ALA			27.861	23.621	29.534	1.00 21.59	A
	ATOM	1889	CA	ALA			28.792	23.848	28.432	1.00 20.02	
											A
	MOTA	1890	СВ	ALA			28.056	23.856	27.106	1.00 18.80	A
45	ATOM	1891	С	ALA			29.481	25.191	28.662	1.00 21.41	A
	ATOM	1892	0	ALA	Α	309	30.680	25.335	28.427	1.00 21.39	A
	ATOM	1893	N	ARG	Α	310	28.717	26.179	29.121	1.00 21.39	A
	ATOM	1894	CA	ARG			29.290	27.494	29.388	1.00 22.02	А
	ATOM	1895	СВ	ARG			28.213	28.479	29.854	1.00 22.39	A
50											
50	ATOM	1896	CG	ARG			28.806	29.756	30.436	1.00 25.30	A -
	MOTA	1897	CD	ARG			27.780	30.852	30.664	1.00 28.33	A
	ATOM	1898	NE	ARG	Α	310	28.420	32.039	31.230	1.00 30.18	A
	MOTA	1899	CZ	ARG	Α	310	27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900	NH1	ARG	Α	310	26.719	33.477	30.634	1.00 31.19	А
55	ATOM	1901		ARG			28.567	34.277	31.742	1.00 30.49	A
23	ATOM	1902	C	ARG			30.376	27.388	30.458	1.00 21.65	A
	ATOM	1903	0	ARG			31.464	27.949	30.311	1.00 20.36	A
	ATOM	1904	N	ASP			30.074	26.677	31.541	1.00 19.57	A
	MOTA	1905	CA	ASP	Α	311	31.043	26.512	32.615	1.00 20.18	A

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	ATOM	1906	СВ		311	30.460	25.649	33.739	1.00 20.39	A
	MOTA	1907	CG	ASP Z	311	31.439	25.446	34.881	1.00 23.35	A
	ATOM	1908	OD1	ASP Z	311	32.158	24.428	34.885	1.00 24.91	A
	ATOM	1909	OD2	ASP Z	311	31.500	26.312	35.776	1.00 26.96	A
5	ATOM	1910	С		A 311	32.322	25.877	32.073	1.00 19.73	A
J	ATOM	1911	0		311	33.422	26.289	32.439	1.00 19.30	A
		1912					24.891	31.188		
	ATOM		N		312	32.179			1.00 16.32	A
	ATOM	1913	CA		A 312	33.349	24.226	30.611	1.00 16.66	A
	ATOM	1914	СВ		312	32.927	23.035	29.744	1.00 16.12	A
10	ATOM	1915	CG	LEU Z	312	34.050	22.320	28.974	1.00 14.73	A
	ATOM	1916	CD1	LEU Z	312	35.192	21.935	29.912	1.00 14.56	A
	MOTA	1917	CD2	LEU Z	312	33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	С	LEU A	312	34.181	25.189	29.774	1.00 16.61	A
	ATOM	1919	0		312	35.402	25.241	29.910	1.00 16.20	А
15	ATOM	1920	N		313	33.515	25.949	28.908	1.00 16.20	A
13	ATOM	1921	CA		1 313	34.207	26.907	28.058	1.00 15.37	A
	ATOM	1922	СВ		313	33.216	27.648	27.130	1.00 16.42	A
	MOTA	1923		VAL Z		33.915	28.796	26.426	1.00 16.93	A
	ATOM	1924	CG2	VAL Z		32.644	26.672	26.103	1.00 17.88	A
20	ATOM	1925	С	VAL Z	313	34.960	27.923	28.911	1.00 17.39	A
	MOTA	1926	0	VAL 2	313	36.093	28.294	28.591	1.00 18.00	A
	MOTA	1927	N	GLU Z	314	34.342	28.364	30.004	1.00 17.61	A
	ATOM	1928	CA	GLU Z	314	34.986	29.331	30.885	1.00 20.43	А
	ATOM	1929	СВ		314	34.009	29.816	31.959	1.00 22.14	A
25	ATOM	1930	CG		314	32.800	30.550	31.396	1.00 26.52	A
23	ATOM	1931	CD		1 314	31.852	31.025	32.478	1.00 20.32	A
	ATOM	1932		GLU A		31.580	30.246	33.417	1.00 33.48	A
	ATOM	1933		GLU Z		31.370	32.173	32.387	1.00 34.81	A
	ATOM	1934	С		314	36.217	28.721	31.539	1.00 19.15	A
30	MOTA	1935	0	GLU Z	314	37.134	29.433	31.934	1.00 21.47	A
	ATOM	1936	N	LYS A	315	36.245	27.400	31.651	1.00 19.51	A
	ATOM	1937	CA	LYS Z	315	37.394	26.749	32.258	1.00 19.17	A
	ATOM	1938	СВ		315	36.946	25.514	33.043	1.00 18.84	A
	ATOM	1939	CG		315	36.280	25.885	34.368	1.00 19.62	A
35	ATOM	1940	CD		315	35.653	24.696	35.073	1.00 19.22	A
33	ATOM	1941	CE		A 315	35.070	25.095	36.427	1.00 21.00	A
	ATOM	1942	ΝZ		315	36.119	25.552	37.381	1.00 19.53	A
	ATOM	1943	С		1 315	38.452	26.393	31.218	1.00 18.96	A
	ATOM	1944	0		315	39.511	25.873	31.561	1.00 19.85	A
40	ATOM	1945	N		316	38.164	26.691	29.950	1.00 17.08	A
	MOTA	1946	CA	LEU Z	316	39.102	26.429	28.854	1.00 16.41	A
	ATOM	1947	CB	LEU Z	316	38.414	25.636	27.738	1.00 13.81	A
	ATOM	1948	CG	LEU Z	316	38.028	24.201	28.115	1.00 14.39	A
	ATOM	1949	CD1	LEU Z		37.139	23.597	27.031	1.00 12.38	А
45	ATOM	1950		LEU Z		39.302	23.373	28.309	1.00 12.77	А
	ATOM	1951	C		316	39.652	27.743	28.290	1.00 17.12	A
					A 316					
	MOTA	1952	0			40.851	27.860	28.023	1.00 16.53	A
	ATOM	1953	N		317	38.780	28.729	28.105	1.00 16.27	A
	ATOM	1954	CA		317	39.228	30.022	27.596	1.00 17.52	A
5 0	ATOM	1955	СВ		317	38.083	30.752	26.887	1.00 16.37	A
	MOTA	1956	CG	LEU Z	317	37.448	29.973	25.727	1.00 18.81	A
	MOTA	1957	CD1	LEU Z	A 317	36.415	30.851	25.018	1.00 16.47	A
	ATOM	1958		LEU Z		38.528	29.526	24.741	1.00 17.87	A
	ATOM	1959	С		A 317	39.745	30.841	28.774	1.00 18.27	A
55	ATOM	1960	0		317	39.078	31.753	29.273	1.00 18.58	A
55	ATOM	1961	N		A 318	40.937	30.475	29.229	1.00 18.02	A
	ATOM	1962	CA	VAL		41.593	31.141	30.342	1.00 18.85	A
	ATOM	1963	СВ		318	41.846	30.153	31.500	1.00 19.91	A
	ATOM	1964	CG1	VAL 2	4 318	42.590	30.848	32.634	1.00 20.01	A

	ATOM	1965	CG2	VAL			40.520	29.584	31.990	1.00 19.44	
	MOTA	1966	С	VAL	Α	318	42.923	31.657	29.811	1.00 19.67	A
	ATOM	1967	0	VAL	Α	318	43.690	30.902	29.208	1.00 18.26	5 A
	ATOM	1968	N	LEU	Α	319	43.197	32.939	30.028	1.00 20.07	A
5	MOTA	1969	CA	LEU	Α	319	44.436	33.533	29.538	1.00 20.98	3 A
	ATOM	1970	СВ	LEU	Α	319	44.521	35.002	29.968	1.00 21.64	l A
	ATOM	1971	CG	LEU	Α	319	43.418	35.908	29.408	1.00 24.38	3 A
	ATOM	1972	CD1	LEU	Α	319	43.606	37.332	29.935	1.00 23.28	3 A
	ATOM	1973	CD2	LEU	Α	319	43.453	35.887	27.875	1.00 24.33	B A
10	ATOM	1974	С	LEU	Α	319	45.680	32.774	29.994	1.00 20.38	3 A
	ATOM	1975	0	LEU	Α	319	46.568	32.496	29.192	1.00 21.34	l A
	MOTA	1976	N	ASP	Α	320	45.742	32.440	31.280	1.00 20.22	2 A
	MOTA	1977	CA	ASP	Α	320	46.879	31.707	31.833	1.00 20.90) A
	ATOM	1978	СВ	ASP	Α	320	46.842	31.760	33.365	1.00 20.76	5 A
15	ATOM	1979	CG	ASP	Α	320	48.049	31.102	34.004	1.00 21.51	A
	MOTA	1980	OD1	ASP	Α	320	48.669	30.226	33.367	1.00 23.46	5 A
	ATOM	1981	OD2	ASP	Α	320	48.371	31.450	35.159	1.00 23.89) A
	MOTA	1982	С	ASP	Α	320	46.814	30.247	31.367	1.00 20.06	5 A
	ATOM	1983	0	ASP	Α	320	45.988	29.476	31.840	1.00 20.54	l A
20	MOTA	1984	N	ALA	Α	321	47.700	29.876	30.451	1.00 20.68	3 A
	MOTA	1985	CA	ALA	Α	321	47.733	28.522	29.903	1.00 22.04	l A
	MOTA	1986	СВ	ALA			48.860	28.411	28.881	1.00 20.75	5 A
	ATOM	1987	С	ALA			47.858	27.400	30.940	1.00 21.62	
	MOTA	1988	0	ALA			47.482	26.259	30.665	1.00 21.99	
25	ATOM	1989	N	THR			48.372	27.715	32.127	1.00 20.89	
	MOTA	1990	CA	THR			48.531	26.698	33.167	1.00 20.82	
	MOTA	1991	СВ	THR			49.670	27.051	34.146	1.00 19.47	
	MOTA	1992		THR			49.341	28.253	34.848	1.00 20.19	
	MOTA	1993		THR			50.981	27.249	33.394	1.00 21.59	
30	ATOM	1994	С	THR			47.264	26.498	33.983	1.00 19.55	
	MOTA	1995	0	THR			47.235	25.673	34.894	1.00 21.13	
	ATOM	1996	N	LYS			46.216	27.248	33.661	1.00 19.33	
	ATOM	1997	CA	LYS			44.962	27.122	34.392	1.00 21.20	
	MOTA	1998	СВ	LYS			44.580	28.460	35.030	1.00 23.75	
35	ATOM	1999	CG	LYS			45.562	28.933	36.084	1.00 28.45	
	ATOM	2000	CD	LYS			45.055	30.177	36.799	1.00 33.76	
	ATOM	2001	CE			323	46.087	30.678	37.802	1.00 36.15	
	ATOM	2002	NΖ	LYS			46.532	29.569	38.693	1.00 37.34	
40	ATOM	2003	С	LYS			43.806	26.614	33.539	1.00 20.68	
40	ATOM	2004	0	LYS			42.649	26.757	33.915	1.00 20.42	
	ATOM	2005	N	ARG			44.114	26.019	32.392	1.00 19.97	
	ATOM	2006	CA	ARG			43.060	25.494	31.531	1.00 17.98	
	ATOM	2007	CB	ARG			43.461	25.609	30.061	1.00 15.95	
15	ATOM	2008	CG	ARG			43.534	27.050	29.603	1.00 17.34	
45	ATOM	2009	CD	ARG			43.996	27.194	28.172	1.00 19.80	
	ATOM	2010	NE	ARG			44.438	28.565	27.944	1.00 16.93	
	ATOM	2011	CZ	ARG ARG			45.410 46.045	28.908	27.108	1.00 19.88	
	ATOM	2012		ARG				27.978 30.181	26.398	1.00 14.58	
50	ATOM ATOM	2013 2014	ип∠ С	ARG			45.774 42.762	24.046	27.015 31.883	1.00 16.51 1.00 18.32	
50	ATOM	2014	0	ARG			43.673	23.222	32.006	1.00 18.32	
	ATOM	2015	N	LEU			41.479	23.748	32.055	1.00 18.32	
	ATOM	2017	CA	LEU			41.050	22.403	32.395	1.00 17.79	
	ATOM	2017	CB	LEU			39.523	22.335	32.425	1.00 17.73	
55	ATOM	2010	CG	LEU			38.896	21.125	33.116	1.00 17.03	
55	ATOM	2020		LEU			39.392	21.123	34.557	1.00 15.93	
	ATOM	2020		LEU			37.375	21.255	33.084	1.00 16.56	
	ATOM	2021	C			325	41.599	21.433	31.356	1.00 18.68	
	ATOM	2023	0			325	41.347	21.586	30.157	1.00 18.28	
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	ATOM	2024	N	GLY	Α	326	42.354	20.439	31.821	1.00	18.18	A
	ATOM	2025	CA	GLY	7	326	42.931	19.462	30.915	1 00	16.36	А
	ATOM	2026	С	GLY			44.443	19.558	30.807		19.15	A
	ATOM	2027	0	GLY	Α	326	45.093	18.592	30.404	1.00	19.52	A
5	ATOM	2028	N	CYS	7	327	45.016	20.708	31.161	1 00	18.16	А
5												
	ATOM	2029	CA	CYS			46.463	20.867	31.075		19.30	A
	ATOM	2030	СВ	CYS	Α	327	46.856	22.350	31.058	1.00	20.22	A
	ATOM	2031	SG	CYS	Α	327	46.782	23.200	32.649	1.00	21.97	Α
	ATOM	2032	С	CYS			47.169	20.157	32.228		20.22	А
10												
10	ATOM	2033	0	CYS			46.561	19.828	33.246		17.92	А
	ATOM	2034	N	GLU	Α	328	48.463	19.933	32.053	1.00	20.51	Α
	ATOM	2035	CA	GLU	Α	328	49.274	19.244	33.042	1.00	23.34	Α
	ATOM	2036	СВ	GLU			50.710	19.139	32.507		28.68	А
	ATOM	2037	CG	GLU			50.754	18.367	31.175		38.24	А
15	ATOM	2038	CD	GLU	Α	328	52.067	18.500	30.414	1.00	43.23	A
	ATOM	2039	OE1	GLU	Α	328	52.535	19.643	30.218	1.00	46.22	Α
	ATOM	2040		GLU			52.618	17.459	29.991		44.90	A
	ATOM	2041	С	GLU			49.234	19.876	34.435		22.11	А
	ATOM	2042	0	GLU	Α	328	49.147	19.161	35.437	1.00	20.27	Α
20	ATOM	2043	N	GLU	Α	329	49.276	21.204	34.506	1.00	18.40	Α
	ATOM	2044	CA	GLU			49.248	21.875	35.801		20.13	A
	ATOM	2045	СВ	GLU			49.587	23.363	35.657		20.36	А
	ATOM	2046	CG	GLU	Α	329	51.014	23.651	35.190	1.00	24.05	Α
	ATOM	2047	CD	GLU	Α	329	51.191	23.518	33.688	1.00	25.93	Α
25	ATOM	2048		GLU			50.213	23.154	32.995		26.61	A
23												
	ATOM	2049	OE2	GLU	А	329	52.311	23.781	33.198	1.00	27.19	A
	ATOM	2050	С	GLU	Α	329	47.890	21.718	36.480	1.00	19.36	Α
	ATOM	2051	0	GLU	Α	329	47.775	21.879	37.694	1.00	18.74	A
• •	ATOM	2052	N	MET			46.863	21.415	35.691		17.28	A
30	ATOM	2053	CA	MET	Α	330	45.520	21.220	36.229	1.00	16.38	Α
	ATOM	2054	CB	MET	Α	330	44.474	21.833	35.294	1.00	17.65	Α
	ATOM	2055	CG	MET	Δ	330	44.460	23.365	35.311		22.95	А
		2056		MET			44.186				26.78	
	ATOM		SD					24.026	36.979			A
	ATOM	2057	CE	MET	Α	330	42.435	23.712	37.186	1.00	24.69	Α
35	ATOM	2058	С	MET	Α	330	45.257	19.730	36.422	1.00	14.30	Α
	ATOM	2059	0	MET	Δ	330	44.127	19.304	36.629	1 00	15.39	А
	ATOM	2060	N	GLU			46.327	18.949	36.346		15.60	A
	MOTA	2061	CA	GLU	Α	331	46.289	17.501	36.531	1.00	17.08	Α
	ATOM	2062	СВ	GLU	Α	331	45.607	17.155	37.862	1.00	17.00	A
40	ATOM	2063	CG	GLU	Δ	331	46.070	18.027	39.038		17.46	А
	ATOM	2064	CD	GLU			47.591	18.179	39.145		20.16	A
	ATOM	2065	OET	GLU	А	331	48.034	19.073	39.896		21.39	A
	ATOM	2066	OE2	GLU	Α	331	48.345	17.420	38.500	1.00	18.87	Α
	ATOM	2067	С	GLU	A	331	45.697	16.658	35.398	1.00	17.80	A
45	ATOM	2068	0	GLU			45.107	15.602	35.636		20.40	A
45												
	ATOM	2069	N	GLY	А	332	45.844	17.133	34.167		16.23	A
	ATOM	2070	CA	GLY	Α	332	45.420	16.353	33.015	1.00	14.10	A
	ATOM	2071	С	GLY	Α	332	43.982	16.154	32.596	1.00	13.54	Α
	ATOM	2072	0	GLY			43.063	16.864	33.017		11.96	A
50												
50	ATOM	2073	N	TYR	А	333	43.804	15.141	31.750	1.00	14.37	А
	ATOM	2074	CA	TYR	Α	333	42.510	14.806	31.182	1.00	13.56	A
	ATOM	2075	СВ	TYR	Α	333	42.722	13.892	29.968	1.00	15.00	Α
	ATOM	2076	CG	TYR			43.153	14.683	28.752		16.46	
												A
	ATOM	2077		TYR			42.206	15.172	27.849		15.29	А
55	ATOM	2078	CE1	TYR	Α	333	42.573	16.002	26.794	1.00	13.42	A
	ATOM	2079		TYR			44.490	15.039	28.561		14.91	А
	ATOM	2080		TYR			44.872	15.877	27.499		14.87	A
	ATOM	2081	CZ	TYR			43.902	16.353	26.626		15.61	А
	ATOM	2082	OH	TYR	Α	333	44.244	17.197	25.599	1.00	17.29	А

	ATOM	2083	С	TYR	Α	333	41.470	14.230	32.127	1.00 1	15.23	A
	ATOM	2084	0	TYR	Δ.	333	40.278	14.323	31.846	1.00 1	16 63	Α
	ATOM	2085	N	GLY			41.907	13.650	33.244	1.00		Α
	ATOM	2086	CA	GLY	Α	334	40.957	13.100	34.202	1.00	L5.07	Α
5	ATOM	2087	С	GLY	Δ	334	39.925	14.146	34.616	1.00 1	16 40	Α
,		2088					38.724			1.00		
	MOTA		0	GLY				13.946	34.433			A
	ATOM	2089	N	PRO	Α	335	40.366	15.278	35.184	1.00 1	L4.96	Α
	ATOM	2090	CD	PRO	Α	335	41.727	15.531	35.689	1.00 1	15.88	Α
	ATOM	2091	CA	PRO			39.444	16.339	35.606	1.00		A
1.0												
10	ATOM	2092	СВ	PRO	А	335	40.383	17.397	36.178	1.00 1	13.19	Α
	ATOM	2093	CG	PRO	Α	335	41.485	16.569	36.758	1.00	13.81	Α
	ATOM	2094	С	PRO	Α	335	38.594	16.877	34.448	1.00 1	15.84	Α
		2095		PRO			37.423			1.00		
	ATOM		0					17.204	34.631			A
	MOTA	2096	N	LEU	Α	336	39.184	16.971	33.257	1.00	16.12	Α
15	ATOM	2097	CA	LEU	Α	336	38.450	17.465	32.094	1.00 1	15.52	Α
	ATOM	2098	СВ	LEU	Δ	336	39.396	17.653	30.898	1.00 1		Α
	MOTA	2099	CG	LEU			38.770	17.991	29.538	1.00 1		А
	ATOM	2100	CD1	LEU	Α	336	37.836	19.182	29.662	1.00 1	L1.25	Α
	ATOM	2101	CD2	LEU	Α	336	39.884	18.285	28.528	1.00 1	14.11	Α
20	ATOM	2102	C	LEU			37.321	16.508	31.714	1.00 1		A
20												
	ATOM	2103	0	LEU			36.176	16.921	31.540	1.00 1		Α
	ATOM	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00 1	L7.22	Α
	ATOM	2105	CA	LYS	Α	337	36.624	14.243	31.235	1.00 1	17.39	Α
	ATOM	2106	СВ	LYS			37.293	12.900	30.921	1.00 1		А
25	ATOM	2107	CG	LYS	Α	337	38.170	12.994	29.676	1.00 2	22.31	Α
	ATOM	2108	CD	LYS	Α	337	39.213	11.892	29.592	1.00 2	24.60	Α
	ATOM	2109	CE	LYS	Δ	337	38.620	10.560	29.189	1.00 2	24 76	Α
	MOTA	2110	NZ	LYS			39.710	9.560	28.997	1.00 2		Α
	ATOM	2111	С	LYS	Α	337	35.577	14.096	32.342	1.00 1	17.33	Α
30	ATOM	2112	0	LYS	Α	337	34.456	13.652	32.090	1.00 1	L4.42	Α
	ATOM	2113	N	ALA			35.928	14.500	33.559	1.00		A
	ATOM	2114	CA	ALA			34.989	14.395	34.674	1.00 1		Α
	ATOM	2115	CB	ALA	Α	338	35.749	14.167	35.980	1.00 1	L9.68	Α
	ATOM	2116	С	ALA	Α	338	34.095	15.621	34.804	1.00 1	18.83	Α
35		2117	0	ALA			33.252		35.695	1.00 1		
33	ATOM							15.687				A
	ATOM	2118	N	HIS	Α	339	34.262	16.596	33.918	1.00 1	L9.42	Α
	ATOM	2119	CA	HIS	Α	339	33.438	17.796	34.004	1.00 1	L9.28	Α
	ATOM	2120	СВ	HIS	Α	339	33.865	18.819	32.949	1.00 1	19.20	A
				HIS								
4.0	ATOM	2121	CG				33.163	20.134	33.074	1.00 2		A
40	ATOM	2122	CD2	HIS	Α	339	33.549	21.299	33.649	1.00	L8.95	Α
	ATOM	2123	ND1	HIS	Α	339	31.880	20.340	32.612	1.00 1	19.10	Α
	ATOM	2124	CE1	HIS	Δ	339	31.506	21.576	32.896	1.00 2	22 19	A
	ATOM	2125		HIS			32.500	22.179	33.525	1.00 2		A
	ATOM	2126	С	HIS	Α	339	31.957	17.448	33.845	1.00	L9.13	Α
45	ATOM	2127	0	HIS	Α	339	31.597	16.576	33.061	1.00 1	19.52	Α
	ATOM	2128	N	PRO			31.079	18.125	34.606	1.00 1		Α
	ATOM	2129	CD	PRO			31.424	19.119	35.640	1.00 1		Α
	ATOM	2130	CA	PRO	Α	340	29.630	17.900	34.569	1.00 2	20.52	Α
	ATOM	2131	СВ	PRO	Α	340	29.091	19.058	35.396	1.00 2	20.74	Α
50	ATOM	2132	CG	PRO			30.146	19.207	36.454	1.00 1		A
50												
	MOTA	2133	С	PRO			29.000	17.834	33.176	1.00 2		А
	MOTA	2134	0	PRO	Α	340	28.049	17.088	32.955	1.00 2	22.48	Α
	ATOM	2135	N	PHE	Α	341	29.528	18.606	32.237	1.00 2	21.33	Α
	ATOM	2136	CA	PHE			28.985	18.610	30.886	1.00 2		A
<i></i>												
55	MOTA	2137	СВ	PHE			29.739	19.624	30.017	1.00 2		А
	ATOM	2138	CG	PHE	Α	341	29.207	19.740	28.613	1.00 2	23.18	Α
	ATOM	2139	CD1	PHE	Α	341	27.903	20.171	28.382	1.00 2		Α
	ATOM	2140		PHE			30.013	19.431	27.522	1.00 2		A
	MOTA	2141	CEI	PHE	А	341	27.410	20.292	27.082	1.00 2	43.54	Α

	ATOM	2142	CE2	PHE	A	341	29.533	19.548	26.220	1.00 21.83	A
	MOTA	2143	CZ	PHE	Α	341	28.228	19.980	25.998	1.00 23.23	A
	MOTA	2144	С	PHE	Α	341	29.055	17.226	30.237	1.00 21.84	A
	MOTA	2145	0	PHE	Α	341	28.232	16.896	29.389	1.00 20.37	A
5	MOTA	2146	N	PHE	Α	342	30.034	16.422	30.640	1.00 20.51	A
	MOTA	2147	CA	PHE	Α	342	30.221	15.085	30.077	1.00 23.01	A
	MOTA	2148	СВ	PHE	Α	342	31.710	14.809	29.850	1.00 18.00	A
	MOTA	2149	CG	PHE	Α	342	32.398	15.812	28.971	1.00 17.05	A
	MOTA	2150	CD1	PHE	Α	342	32.010	15.987	27.652	1.00 17.78	A
10	MOTA	2151	CD2	PHE	Α	342	33.487	16.534	29.450	1.00 15.72	A
	MOTA	2152		PHE			32.702	16.867	26.811	1.00 18.08	A
	MOTA	2153	CE2	PHE			34.184	17.414	28.617	1.00 17.45	A
	MOTA	2154	CZ	PHE			33.790	17.578	27.298	1.00 16.56	A
	MOTA	2155	С	PHE			29.679	13.972	30.976	1.00 24.95	A
15	MOTA	2156	0	PHE			30.002	12.798	30.777	1.00 23.95	A
	ATOM	2157	N	GLU			28.861	14.333	31.958	1.00 27.35	A
	MOTA	2158	CA	GLU			28.325	13.349	32.897	1.00 30.28	A
	MOTA	2159	СВ			343	27.187	13.964	33.716	1.00 32.20	A
	ATOM	2160	CG			343	26.581	12.991	34.714	1.00 39.71	А
20	ATOM	2161	CD	GLU			25.628	13.661	35.688	1.00 44.72	A
	ATOM	2162		GLU			24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2				25.847	13.526	36.911	1.00 46.89	A
	ATOM	2164	С	GLU			27.852	12.017	32.305	1.00 28.98	A
2.5	ATOM	2165	0			343	28.225	10.952	32.800	1.00 31.73	A
25	ATOM	2166	N	SER			27.037	12.067	31.258	1.00 26.09	A
	ATOM	2167	CA			344	26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168	CB	SER			25.129	11.089	30.067	1.00 28.73	A
	ATOM	2169	OG	SER			25.203	11.942	28.940	1.00 30.91	A
20	ATOM	2170	C	SER			27.407	10.214	29.577	1.00 27.66	A
30	ATOM	2171	0	SER			26.987	9.281	28.900	1.00 28.66	A
	ATOM	2172	N	VAL			28.627	10.715	29.419	1.00 26.75	A
	ATOM	2173	CA	VAL			29.534	10.183	28.402	1.00 23.44	A
	ATOM	2174 2175	CB	VAL		345	30.565 31.589	11.256 10.631	27.950 26.995	1.00 23.10 1.00 22.24	A
35	ATOM	2176		VAL			29.854	12.418	26.995	1.00 22.24	A
33	ATOM ATOM	2176	CGZ			345	30.326	8.957	28.855	1.00 20.03	A A
	ATOM	2178	0	VAL			30.326	8.930	29.960	1.00 24.28	A
	ATOM	2179	N	THR			30.374	7.942	27.997	1.00 22.83	A
	ATOM	2179	CA	THR			31.153	6.740	28.272	1.00 21.77	A
40	ATOM	2181	CB	THR			30.391	5.455	27.857	1.00 26.53	A
40	ATOM	2182		THR			29.248	5.284	28.706	1.00 20.93	A
	ATOM	2183	CG2	THR			31.289	4.231	27.990	1.00 24.28	A
	ATOM	2184	C	THR			32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	0	THR			32.306	6.827	26.160	1.00 24.50	A
45	ATOM	2186	N	TRP			33.508	7.270	28.013	1.00 22.98	A
15	ATOM	2187	CA	TRP			34.744	7.569	27.300	1.00 23.81	A
	ATOM	2188	СВ	TRP			35.683	8.352	28.219	1.00 22.54	A
	ATOM	2189	CG	TRP			35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190		TRP			35.257	10.927	28.040	1.00 19.11	A
50	ATOM	2191		TRP			34.581	11.881	28.838	1.00 18.39	A
	ATOM	2192		TRP			35.878	11.351	26.858	1.00 18.16	А
	ATOM	2193		TRP			34.397	9.883	29.828	1.00 18.35	А
	ATOM	2194		TRP			34.065	11.218	29.923	1.00 19.51	А
	ATOM	2195		TRP			34.510	13.234	28.491	1.00 16.88	A
55	ATOM	2196		TRP			35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197		TRP			35.127	13.624	27.327	1.00 18.16	А
	ATOM	2198	С	TRP			35.538	6.429	26.675	1.00 25.79	А
	ATOM	2199	0	TRP			36.304	6.654	25.742	1.00 24.67	A
	ATOM	2200	N	ALA	Α	348	35.360	5.215	27.183	1.00 27.10	А

	MOTA	2201	CA	ALA A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	СВ	ALA A	348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	С	ALA A		35.895	3.620	25.256	1.00 27.18	A
	MOTA	2204	0	ALA A	348	36.830	3.148	24.613	1.00 29.41	A
5	ATOM	2205	N	ASN A	349	34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN A		34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	СВ	ASN A	349	33.700	1.962	23.444	1.00 29.37	A
	MOTA	2208	CG	ASN A	349	32.299	2.088	24.013	1.00 30.92	A
	ATOM	2209	OD1	ASN A	349	32.045	2.942	24.859	1.00 30.17	A
10	ATOM	2210		ASN A		31.386	1.237	23.553	1.00 33.52	А
10										
	ATOM	2211	С	ASN A		33.599	4.265	22.509	1.00 26.47	A
	MOTA	2212	0	ASN A	349	32.669	3.843	21.819	1.00 25.87	A
	ATOM	2213	N	LEU A	350	33.947	5.543	22.518	1.00 24.45	A
	ATOM	2214	CA	LEU A	350	33.203	6.510	21.721	1.00 23.14	А
1.5										
15	ATOM	2215	СВ	LEU P		33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU P	350	33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217	CD1	LEU A	350	34.646	9.756	23.293	1.00 19.36	A
	ATOM	2218		LEU A		32.220	9.094	23.319	1.00 18.78	А
	ATOM	2219	С	LEU P		33.082	6.152	20.240	1.00 22.60	A
20	MOTA	2220	0	LEU P	350	32.011	6.296	19.650	1.00 21.15	A
	ATOM	2221	N	HIS A	351	34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS A		34.089	5.387	18.204	1.00 27.83	А
	ATOM	2223	СВ	HIS A		35.506	5.325	17.596	1.00 29.36	A
	MOTA	2224	CG	HIS F	351	36.082	3.950	17.493	1.00 32.07	A
25	ATOM	2225	CD2	HIS A	351	36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226	ND1	HIS A	351	36.197	3.285	16.291	1.00 33.02	A
									1.00 33.58	
	ATOM	2227		HIS A		36.775	2.113	16.493		A
	ATOM	2228	NE2	HIS A	351	37.036	1.992	17.782	1.00 31.76	A
	ATOM	2229	С	HIS A	351	33.258	4.144	17.874	1.00 28.12	A
30	ATOM	2230	0	HIS A	351	33.015	3.847	16.707	1.00 29.49	A
	ATOM	2231		GLN A		32.800	3.442	18.908	1.00 29.28	A
			N							
	ATOM	2232	CA	GLN A		31.963	2.255	18.726	1.00 29.67	A
	ATOM	2233	CB	GLN A	352	32.366	1.145	19.694	1.00 30.56	A
	ATOM	2234	CG	GLN A	352	33.169	0.041	19.041	1.00 30.88	A
35	ATOM	2235	CD	GLN A		34.493	-0.186	19.729	1.00 31.21	A
33										
	ATOM	2236		GLN A		34.541	-0.450	20.928	1.00 30.76	A
	ATOM	2237	NE2	GLN A	352	35.578	-0.084	18.971	1.00 32.30	A
	MOTA	2238	С	GLN A	352	30.504	2.638	18.963	1.00 30.42	A
	ATOM	2239	0	GLN A	352	29.595	1.831	18.770	1.00 29.01	A
40							3.875		1.00 27.64	
40	ATOM	2240	N	GLN A		30.290		19.397		A
	MOTA	2241	CA	GLN A	353	28.948	4.365	19.652	1.00 27.42	A
	MOTA	2242	СВ	GLN A	353	28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG	GLN A	353	29.408	4.837	22.115	1.00 27.34	A
	ATOM	2244	CD	GLN A		29.638	5.914	23.156	1.00 27.19	A
4.5										
45	ATOM	2245		GLN A		28.875	6.872	23.252	1.00 28.29	A
	MOTA	2246	NE2	GLN A	353	30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	С	GLN A	353	28.375	4.989	18.385	1.00 29.00	A
	ATOM	2248	0	GLN A		29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR A		27.053	4.984	18.276	1.00 27.31	A
50	ATOM	2250	CA	THR P	354	26.390	5.568	17.119	1.00 27.85	A
	ATOM	2251	СВ	THR A	354	24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.07	A
	ATOM	2253		THR A		24.289	5.585	15.709	1.00 29.58	A
	ATOM	2254	С	THR A	354	26.244	7.062	17.376	1.00 26.85	A
55	MOTA	2255	0	THR A	354	25.592	7.475	18.329	1.00 25.77	А
	ATOM	2256	N	PRO F		26.867	7.898	16.533	1.00 27.22	А
	ATOM	2257	CD	PRO F		27.792	7.588	15.431	1.00 25.89	A
	ATOM	2258	CA	PRO P	355	26.763	9.346	16.734	1.00 27.23	A
	ATOM	2259	СВ	PRO A	355	27.625	9.915	15.609	1.00 24.91	A

	ATOM	2260	CG	PRO	Α	355	28.643	8.838	15.385	1.00	25.54		A
	MOTA	2261	С	PRO			25.322	9.837	16.641		28.07		А
	ATOM	2262	0	PRO			24.548	9.364	15.810		27.24		A
	ATOM	2263	N	PRO			24.941	10.792	17.500		28.28		A
5				PRO			25.752		18.462		28.31		
3	ATOM	2264	CD					11.560					A
	MOTA	2265	CA	PRO			23.572	11.306	17.448		28.44		A
	MOTA	2266	СВ	PRO			23.539	12.301	18.604		28.11		A
	ATOM	2267	CG	PRO	Α	356	24.946	12.832	18.612	1.00	26.86		Α
	ATOM	2268	С	PRO	Α	356	23.363	11.978	16.097	1.00	29.25		Α
10	ATOM	2269	0	PRO	Α	356	24.304	12.537	15.529	1.00	27.27		Α
	ATOM	2270	N	ALA			22.143	11.910	15.575	1.00	30.45		Α
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00	32.81		А
	ATOM	2272	СВ	ALA			20.507	12.019	13.757		31.99		A
		2273	С	ALA			21.824	14.035	14.448		35.05		A
1.5	ATOM												
15	ATOM	2274	0	ALA			21.194	14.561	15.369		35.04		A
	ATOM	2275	N	LEU			22.516	14.730	13.552		37.81		A
	ATOM	2276	CA	LEU	Α	358	22.578	16.185	13.597	1.00	42.15		А
	ATOM	2277	СВ	LEU	Α	358	23.679	16.681	12.658	1.00	39.54		Α
	ATOM	2278	CG	LEU	Α	358	25.086	16.285	13.109	1.00	39.51		Α
20	ATOM	2279	CD1	LEU	Α	358	26.102	16.686	12.062	1.00	39.29		Α
	ATOM	2280	CD2	LEU	Α	358	25.395	16.953	14.445	1.00	40.01		Α
	ATOM	2281	С	LEU			21.241	16.837	13.242		45.91		A
	ATOM	2282	0	LEU			20.874	16.927	12.069		45.71		A
25	ATOM	2283	N	THR			20.530	17.290	14.275		50.06		A
25	ATOM	2284	CA	THR			19.223	17.939	14.140		53.73		A
	MOTA	2285	СВ	THR			19.353	19.428	13.726		54.04		Α
	ATOM	2286	OG1	THR	Α	359	19.995	19.521	12.448	1.00	56.35		А
	ATOM	2287	CG2	THR	Α	359	20.158	20.204	14.763	1.00	54.32		A
	MOTA	2288	С	THR	Α	359	18.309	17.236	13.139	1.00	54.47		A
30	ATOM	2289	0	THR	Α	359	18.483	16.016	12.930	1.00	55.90		Α
	ATOM	2290	OXT	THR	Α	359	17.407	17.908	12.595	1.00	56.97		A
	TER												
	ATOM	1	СВ	PRO	B	71	99.838	54.646	-7.659	1 00	20.00	6	
	ATOM	2	CG	PRO		71	99.216	55.105	-6.341		20.00	6	
35	ATOM	3	C			71	98.903	54.776	-9.981		20.00		
33				PRO								6	
	ATOM	4	0	PRO		71	98.022		-10.109		20.00	8	
	MOTA	5	N	PRO		71	97.782	55.851	-8.042		20.00	7	
	MOTA	6	CD	PRO	В	71	97.728	55.323	-6.668	1.00	20.00	6	
	ATOM	7	CA	PRO	В	71	99.087	55.515	-8.658	1.00	20.00	6	
40	ATOM	8	N	PRO	В	72	99.732	55.097	-10.985	1.00	20.00	7	
	ATOM	9	CD	PRO	В	72	100.794	56.121	-10.977	1.00	20.00	6	
	ATOM	10	CA	PRO	В	72	99.645	54.451	-12.297	1.00	20.00	6	
	ATOM	11	СВ	PRO		72			-13.017		20.00	6	
	ATOM	12	CG	PRO		72	101.026		-12.456		20.00	6	
45	ATOM	13	C	PRO		72	99.627		-12.202		20.00	6	
73													
	ATOM	14	0	PRO		72	100.246		-11.314		20.00	8	
	ATOM	15	N	ALA		73	98.906		-13.122		20.00	7	
	ATOM	16	CA	ALA		73	98.805		-13.167		20.00	6	
	ATOM	17	СВ	ALA	В	73	97.420	50.392	-12.710	1.00	20.00	6	
50	ATOM	18	С	ALA	В	73	99.053	50.398	-14.604	1.00	20.00	6	
	ATOM	19	0	ALA	В	73	99.027	51.215	-15.526	1.00	20.00	8	
	ATOM	20	N	PRO	В	74	99.313	49.100	-14.818	1.00	20.00	7	
	ATOM	21	CD	PRO		74	99.473		-13.857		20.00	6	
	ATOM	22	CA	PRO		74	99.553		-16.189		20.00	6	
55	ATOM	23	CB	PRO		74	99.700		-16.023		20.00	6	
55													
	ATOM	24	CG	PRO		74	100.292		-14.649		20.00	6	
	ATOM	25	C	PRO		74	98.371		-17.079		20.00	6	
	ATOM	26	0	PRO		74			-16.583		20.00	8	
	MOTA	27	N	ALA	В	75	98.589	49.037	-18.389	1.00	20.00	7	

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28
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                                               49.368 -19.321
                                                                1.00 20.00
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                                                49.462 -20.745
                                                                 1.00 20.00
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                       ALA B
                                                                              6
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                   С
                                       96.446
                                                                 1.00 20.00
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                               75
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	ATOM	90	CD2	PHE	В	82	94.525	38.423 -22.961	1.00 20.00 6
5	ATOM	91	CE1	PHE	В	82	95.976	37.479 -20.793	1.00 20.00 6
_	ATOM	92	CE2	PHE		82	94.615	39.188 -21.800	1.00 20.00 6
	ATOM	93	CZ	PHE		82	95.343	38.712 -20.713	1.00 20.00 6
	ATOM	94	С	PHE		82	95.929	35.719 -26.496	1.00 20.00 6
10	ATOM	95	0	PHE		82	95.342	36.061 -27.524	1.00 20.00 8
10	ATOM	96	N	LYS		83	96.406	34.500 -26.286	1.00 20.00 7
	MOTA	97	CA	LYS	В	83	96.242	33.411 -27.228	1.00 20.00 6
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	ATOM	99	CG	LYS	В	83	97.503	31.531 -28.425	1.00 20.00 6
	ATOM	100	CD	LYS	В	83	98.888	31.074 -28.856	1.00 20.00 6
15	ATOM	101	CE	LYS		83	98.826	29.808 -29.699	1.00 20.00 6
15	ATOM	102	ΝZ	LYS		83	98.287	28.654 -28.918	1.00 20.00 7
	ATOM	103	C	LYS		83	95.387	32.446 -26.416	
	ATOM	104	0	LYS		83	95.884	31.776 -25.510	1.00 20.00 8
	ATOM	105	N	PHE	В	8 4	94.094	32.393 -26.710	1.00 20.00 7
20	ATOM	106	CA	PHE	В	8 4	93.217	31.511 -25.958	1.00 20.00 6
	MOTA	107	СВ	PHE	В	84	91.758	31.928 -26.133	1.00 20.00 6
	ATOM	108	CG	PHE	В	84	91.426	33.228 -25.462	1.00 20.00 6
	ATOM	109	CD1	PHE	В	84	91.668	34.439 -26.099	1.00 20.00 6
	ATOM	110		PHE		8 4	90.907	33.243 -24.174	1.00 20.00 6
25	ATOM	111		PHE		84	91.400	35.644 -25.464	1.00 20.00 6
23	ATOM	112	CE2	PHE		84	90.636	34.447 -23.528	1.00 20.00 6
	ATOM	113	CZ	PHE		84	90.884	35.646 -24.176	1.00 20.00 6
	ATOM	114	С	PHE		8 4	93.402	30.054 -26.335	1.00 20.00 6
	ATOM	115	0	PHE		84	93.734	29.734 -27.476	1.00 20.00 8
30	ATOM	116	N	GLY	В	85	93.196	29.178 -25.359	1.00 20.00 7
	MOTA	117	CA	$\operatorname{GL} Y$	В	85	93.349	27.758 -25.591	1.00 20.00 6
	ATOM	118	С	GLY	В	85	92.103	26.977 -25.221	1.00 20.00 6
	ATOM	119	0	GLY	В	85	90.982	27.393 -25.525	1.00 20.00 8
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35	ATOM	121	CA	LYS		86	91.182	25.005 -24.153	1.00 20.00 6
55	ATOM	122	CB	LYS		86	91.695	23.640 -23.687	1.00 20.00 6
						86		23.667 -22.356	1.00 20.00 6
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	ATOM	124	CD	LYS		86	92.855	22.272 -21.941	1.00 20.00 6
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40	ATOM	126	NZ	LYS		86	94.209	20.975 -20.287	1.00 20.00 7
	MOTA	127	С	LYS	В	86	90.267	25.576 -23.077	1.00 20.00 6
	MOTA	128	0	LYS	В	86	90.668	26.410 -22.260	1.00 20.00 8
	ATOM	129	N	ILE	В	87	89.026	25.106 -23.102	1.00 20.00 7
	ATOM	130	CA	ILE	В	87	88.023	25.497 -22.131	1.00 20.00 6
45	ATOM	131	СВ	ILE		87	86.604	25.159 -22.647	1.00 20.00 6
	ATOM	132		ILE		87	85.582	25.261 -21.503	1.00 20.00 6
	ATOM	133		ILE		87	86.260	26.085 -23.820	
				ILE					
	ATOM	134				87	84.912	25.819 -24.463	1.00 20.00 6
50	ATOM	135	С	ILE		87	88.312	24.687 -20.872	1.00 20.00 6
50	ATOM	136	0	ILE		87	88.396	23.461 -20.927	1.00 20.00 8
	ATOM	137	N	LEU		88	88.473	25.368 -19.742	1.00 20.00 7
	ATOM	138	CA	LEU	В	88	88.757	24.686 -18.486	1.00 20.00 6
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	ATOM	140	CG	LEU	В	88	90.968	25.987 -18.112	1.00 20.00 6
55	ATOM	141		LEU		88	91.611	27.006 -17.186	1.00 20.00 6
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	ATOM	143	CDZ	LEU		88	87.471	24.298 -17.776	1.00 20.00 6
	ATOM	144	0	LEU		88	87.434		1.00 20.00 8
	ATOM	145	N	GLY	В	89	86.410	25.051 -18.024	1.00 20.00 7

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                                      74.756
                                                                            7
                                              39.248
                                                      -3.501
                                                               1.00 20.00
    MOTA
             473
                  NH2 ARG B 129
             474
                                      81.354
                                              39.788
                                                              1.00 20.00
    MOTA
                  С
                      ARG B 129
                                                      -6.146
                                                                            6
             475
                                      82.315
                                              39.885
                                                               1.00 20.00
35
    ATOM
                  0
                      ARG B 129
                                                      -5.379
    MOTA
             476
                  Ν
                      GLU B 130
                                      81.316
                                              38.917
                                                      -7.151
                                                               1.00 20.00
                                                                            7
    MOTA
             477
                  CA
                      GLU B 130
                                      82.439
                                              38.029
                                                      -7.421
                                                               1.00 20.00
    MOTA
             478
                      GLU B 130
                                      82.191
                                              37.211
                                                      -8.692
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                  CB
    MOTA
             479
                  CG
                      GLU B 130
                                      83.408
                                              36.427
                                                      -9.167
                                                               1.00 20.00
40
    MOTA
             480
                  CD
                      GLU B 130
                                      83.060
                                              35.338 -10.168
                                                               1.00 20.00
             481
                  OE1 GLU B 130
                                      82.227
                                              35.590 -11.061
                                                               1.00 20.00
    MOTA
                  OE2 GLU B 130
                                      83.626
                                              34.231 -10.068
                                                               1.00 20.00
    ATOM
             482
    MOTA
             483
                  С
                      GLU B 130
                                      83.708
                                              38.853
                                                      -7.580
                                                               1.00 20.00
                                                                            6
             484
                      GLU B 130
                                      84.723
                                              38.575
                                                      -6.940
                                                               1.00 20.00
    MOTA
                  0
             485
                      ARG B 131
                                      83.641
                                              39.874
                                                      -8.428
                                                               1.00 20.00
    MOTA
                  N
                                      84.788
                                              40.742
    MOTA
             486
                  CA
                      ARG B 131
                                                      -8.673
                                                               1.00 20.00
                                                                            6
                                      84.459
    MOTA
             487
                      ARG B 131
                                              41.759
                                                      -9.777
                                                               1.00 20.00
                  СВ
                                                                            6
    MOTA
             488
                  CG
                      ARG B 131
                                      85.580
                                              42.753 -10.035
                                                               1.00 20.00
                                                                            6
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                      ARG B 131
                                      85.262
                                              43.716 -11.167
                                                               1.00 20.00
    ATOM
             490
                      ARG B 131
                                      86.351
                                              44.673 -11.355
                                                               1.00 20.00
                                                                            7
                  NE
                      ARG B 131
                                      86.416
                                              45.561 -12.343
                                                               1.00 20.00
    MOTA
             491
                  CZ
                  NH1 ARG B 131
                                      85.450
                                              45.623 -13.250
                                                               1.00 20.00
                                                                            7
    MOTA
             492
             493
                  NH2 ARG B 131
                                      87.450
                                              46.388 -12.426
                                                               1.00 20.00
                                                                            7
    MOTA
                                      85.228
                                              41.485
                                                      -7.409
    MOTA
             494
                  С
                      ARG B 131
                                                               1.00 20.00
                                                                            6
55
    MOTA
             495
                  0
                      ARG B 131
                                      86.413
                                              41.500
                                                      -7.071
                                                               1.00 20.00
                                                                            8
    MOTA
             496
                  Ν
                      ASP B 132
                                      84.277
                                              42.103
                                                      -6.715
                                                               1.00 20.00
                                                                            7
                      ASP B 132
                                      84.594
    MOTA
             497
                  CA
                                              42.848
                                                      -5.505
                                                              1.00 20.00
                                                                            6
                  СВ
                      ASP B 132
                                                      -4.987
             498
                                      83.350
                                              43.575
                                                              1.00 20.00
    MOTA
                                                                            6
                      ASP B 132
                                      82.865 44.658 -5.943 1.00 20.00
             499
                  CG
    MOTA
                                                                            6
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	7.50.75	F 0 0	OD 1	700	_	1 2 0	0.2 61.0	45 010	6 006	1 00	00 00	0
	ATOM	500		ASP			83.612	45.010	-6.886		20.00	8
	ATOM	501		ASP			81.739	45.167	-5.747		20.00	8
	MOTA	502	С	ASP			85.192	41.969	-4.401		20.00	6
	MOTA	503	0	ASP	В	132	86.191	42.337	-3.783	1.00	20.00	8
5	ATOM	504	N	VAL	В	133	84.596	40.809	-4.150	1.00	20.00	7
	MOTA	505	CA	VAL	В	133	85.131	39.933	-3.116	1.00	20.00	6
	ATOM	506	СВ	VAL	В	133	84.226	38.698	-2.885	1.00	20.00	6
	ATOM	507		VAL			84.920	37.713	-1.957		20.00	6
	ATOM	508		VAL			82.893	39.135	-2.271		20.00	6
10	ATOM	509	C	VAL			86.540	39.470	-3.477		20.00	6
10												
	ATOM	510	0	VAL			87.460	39.602	-2.675		20.00	8
	ATOM	511	N	MET			86.721	38.950	-4.688		20.00	7
	MOTA	512	CA	MET			88.040	38.474	-5.083		20.00	6
	MOTA	513	СВ	MET	В	134	88.004	37.879	-6.492	1.00	20.00	6
15	ATOM	514	CG	MET	В	134	87.183	36.603	-6.573	1.00	20.00	6
	MOTA	515	SD	MET	В	134	87.477	35.650	-8.077	1.00	20.00	16
	ATOM	516	CE	MET	В	134	88.730	34.515	-7.475	1.00	20.00	6
	ATOM	517	С	MET			89.115	39.552	-4.994		20.00	6
	ATOM	518	0	MET			90.253	39.264	-4.626		20.00	8
20			N	SER			88.758		-5.319		20.00	7
20	ATOM	519						40.790				
	ATOM	520	CA	SER			89.708	41.899	-5.260		20.00	6
	MOTA	521	СВ	SER			89.084	43.175	-5.836		20.00	6
	ATOM	522	OG	SER			88.742	43.009	-7.202		20.00	8
	MOTA	523	С	SER	В	135	90.165	42.184	-3.830	1.00	20.00	6
25	MOTA	524	0	SER	В	135	91.228	42.762	-3.614	1.00	20.00	8
	ATOM	525	N	ARG	В	136	89.354	41.782	-2.857	1.00	20.00	7
	ATOM	526	CA	ARG	В	136	89.672	42.013	-1.450	1.00	20.00	6
	ATOM	527	СВ	ARG			88.384	42.156	-0.637		20.00	6
	ATOM	528	CG	ARG			87.509	43.336	-1.018		20.00	6
30		529		ARG				43.306			20.00	6
30	ATOM		CD				86.215		-0.211			
	ATOM	530	NE	ARG			86.491	43.117	1.209		20.00	7
	ATOM	531	CZ	ARG			85.565	42.888	2.132		20.00	6
	MOTA	532		ARG			84.285	42.821	1.786		20.00	7
	MOTA	533	NH2	ARG	В	136	85.920	42.715	3.401	1.00	20.00	7
35	ATOM	534	С	ARG	В	136	90.506	40.891	-0.839	1.00	20.00	6
	MOTA	535	0	ARG	В	136	91.091	41.054	0.231	1.00	20.00	8
	ATOM	536	N	LEU	В	137	90.556	39.752	-1.515	1.00	20.00	7
	ATOM	537	CA	LEU	В	137	91.300	38.609	-1.005		20.00	6
	ATOM	538	СВ	LEU			90.665	37.307	-1.504		20.00	6
40	ATOM	539	CG	LEU			89.172	37.099	-1.213		20.00	6
40	ATOM	540		LEU			88.748	35.728	-1.734		20.00	6
	ATOM	541		LEU			88.897	37.205	0.280		20.00	6
	ATOM	542	С	LEU			92.771	38.648	-1.402		20.00	6
	ATOM	543	0	LEU			93.103	38.871	-2.566		20.00	8
45	ATOM	544	N	ASP	В	138	93.645	38.436	-0.424	1.00	20.00	7
	MOTA	545	CA	ASP	В	138	95.086	38.422	-0.656	1.00	20.00	6
	MOTA	546	CB	ASP	В	138	95.696	39.797	-0.352	1.00	20.00	6
	ATOM	547	CG	ASP	В	138	97.179	39.854	-0.674	1.00	20.00	6
	ATOM	548	OD1	ASP	В	138	97.601	39.173	-1.634		20.00	8
50	ATOM	549		ASP			97.920	40.581	0.022		20.00	8
20	ATOM	550	C	ASP			95.678	37.369	0.263		20.00	6
							96.353		1.243			
	ATOM	551	0	ASP				37.685			20.00	8
	ATOM	552	N	HIS			95.410	36.111	-0.065		20.00	7
	ATOM	553	CA	HIS			95.871	34.984	0.731		20.00	6
55	MOTA	554	СВ	HIS			94.769	34.610	1.737		20.00	6
	ATOM	555	CG	HIS	В	139	95.173	33.561	2.725	1.00	20.00	6
	MOTA	556	CD2	HIS	В	139	95.543	33.657	4.025	1.00	20.00	6
	ATOM	557		HIS			95.241	32.221	2.405		20.00	7
	ATOM	558		HIS			95.635	31.537	3.466		20.00	6
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	ATOM	559	NE2	HIS 1	В	139	95.825	32.385	4.461	1.00 20.	.00	7
	ATOM	560	C	HIS 1	В	139	96.176	33.828	-0.221	1.00 20.	.00	6
	ATOM	561	0	HIS I	R	139	95.444	33.595	-1.182	1.00 20.	.00	8
		562		PRO I		140				1.00 20.		7
_	ATOM		N				97.257	33.080	0.038			
5	ATOM	563	CD	PRO 1	В	140	98.128	33.140	1.225	1.00 20.	.00	6
	ATOM	564	CA	PRO 1	В	140	97.635	31.959	-0.827	1.00 20.	.00	6
	ATOM	565	СВ	PRO I	R	140	98.913	31.433	-0.171	1.00 20.	0.0	6
		566	CG					31.730		1.00 20.		6
	ATOM			PRO 1			98.687		1.277			
	ATOM	567	С	PRO 1	В	140	96.614	30.846	-1.072	1.00 20.	.00	6
10	ATOM	568	0	PRO 1	В	140	96.747	30.107	-2.044	1.00 20.	.00	8
	ATOM	569	N	PHE I	R	141	95.607	30.712	-0.211	1.00 20.	$\cap \cap$	7
	ATOM	570	CA	PHE 1			94.620	29.649	-0.398	1.00 20.		6
	ATOM	571	СВ	PHE 1	В	141	94.206	29.056	0.961	1.00 20.	.00	6
	ATOM	572	CG	PHE I	В	141	95.321	28.335	1.681	1.00 20.	.00	6
15	ATOM	573		PHE 1			96.351	27.716	0.967	1.00 20.		6
13												
	ATOM	574		PHE 1			95.311	28.227	3.067	1.00 20.		6
	ATOM	575	CE1	PHE 1	В	141	97.350	27.000	1.627	1.00 20.	.00	6
	ATOM	576	CE2	PHE 1	В	141	96.307	27.510	3.740	1.00 20.	.00	6
	ATOM	577	CZ	PHE 1			97.328	26.895	3.018	1.00 20.		6
20												
20	ATOM	578	С	PHE 1			93.371	30.063	-1.181	1.00 20.		6
	ATOM	579	0	PHE 1	В	141	92.335	29.398	-1.114	1.00 20.	.00	8
	ATOM	580	N	PHE 1	В	142	93.471	31.150	-1.934	1.00 20.	.00	7
	ATOM	581	CA	PHE 1			92.337	31.625	-2.721	1.00 20.		6
	ATOM	582	СВ	PHE I			91.739	32.883	-2.082	1.00 20.		6
25	ATOM	583	CG	PHE 1	В	142	91.048	32.628	-0.772	1.00 20.	.00	6
	ATOM	584	CD1	PHE 1	В	142	89.715	32.227	-0.740	1.00 20.	.00	6
	ATOM	585	CD2	PHE 1	R	142	91.741	32.747	0.429	1.00 20.	$\cap \cap$	6
	ATOM	586		PHE 1			89.080	31.944	0.472	1.00 20.		6
	ATOM	587	CE2	PHE 1	В	142	91.116	32.465	1.647	1.00 20.	.00	6
30	ATOM	588	CZ	PHE 1	В	142	89.785	32.064	1.667	1.00 20.	.00	6
	ATOM	589	С	PHE 1		142	92.758	31.945	-4.146	1.00 20.		6
	ATOM	590	0	PHE 1			93.865	32.429	-4.371	1.00 20.		8
	ATOM	591	N	VAL I	В	143	91.883	31.653	-5.106	1.00 20.	.00	7
	ATOM	592	CA	VAL I	В	143	92.167	31.960	-6.504	1.00 20.	.00	6
35	ATOM	593	СВ	VAL I	R	143	91.009	31.513	-7.435	1.00 20.	$\cap \cap$	6
55		594		VAL I						1.00 20.		
	ATOM						91.116	32.209	-8.795			6
	ATOM	595	CG2	VAL I	В	143	91.061	30.000	-7.623	1.00 20.	.00	6
	ATOM	596	С	VAL I	В	143	92.301	33.469	-6.545	1.00 20.	.00	6
	ATOM	597	0	VAL I	В	143	91.505	34.179	-5.932	1.00 20.	.00	8
40	ATOM	598	N	LYS			93.312	33.957	-7.252	1.00 20.		7
70												
	ATOM	599	CA	LYS I			93.547	35.392	-7.340	1.00 20.		6
	ATOM	600	СВ	LYS I	В	144	95.051	35.689	-7.267	1.00 20.	.00	6
	ATOM	601	CG	LYS I	В	144	95.382	37.182	-7.318	1.00 20.	.00	6
	ATOM	602	CD	LYS I	R	144	96.881	37.441	-7.201	1.00 20.		6
45										1.00 20.		
43	ATOM	603	CE	LYS I			97.191	38.936	-7.298			6
	ATOM	604	NZ	LYS I	В	144	98.661	39.215	-7.246	1.00 20.	.00	7
	ATOM	605	С	LYS I	В	144	92.989	36.003	-8.614	1.00 20.	.00	6
	ATOM	606	0	LYS I	R	144	92.993	35.371	-9.675	1.00 20.		8
										1.00 20.		
	ATOM	607	N	LEU 1			92.495	37.230	-8.490			7
50	ATOM	608	CA	LEU 1	В	145	91.968	37.975	-9.624	1.00 20.	.00	6
	ATOM	609	СВ	LEU I	В	145	90.678	38.703	-9.234	1.00 20.	.00	6
	ATOM	610	CG	LEU I			89.938	39 486	-10.326	1.00 20.	$\cap \cap$	6
	ATOM	611		LEU I			88.611	39.992	-9.782	1.00 20.		6
	MOTA	612	CD2	LEU 1	В	145	90.791	40.652	-10.806	1.00 20.	.00	6
55	ATOM	613	С	LEU I	В	145	93.059	38.984	-9.968	1.00 20.	.00	6
	ATOM	614	0	LEU I			93.291	39.940	-9.216	1.00 20.		8
	ATOM	615	N	TYR I			93.735		-11.093	1.00 20.		7
	ATOM	616	CA	TYR I	В	146	94.815	39.657	-11.517	1.00 20.	.00	6
	ATOM	617	СВ	TYR I	В	146	95.821	38.904	-12.389	1.00 20.	.00	6

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	ATOM	618	CG	TYR I	3 146	96.624	37.858 -11.661	1.00 20.00	6
	ATOM	619	CD1	TYR I	3 146	96.139	36.559 -11.498	1.00 20.00	6
	ATOM	620	CE1	TYR E	146	96.894	35.589 -10.836	1.00 20.00	6
	ATOM	621		TYR I		97.878	38.165 -11.140	1.00 20.00	6
_									
5	ATOM	622	CE2	TYR I	3 146	98.639	37.208 -10.476	1.00 20.00	6
	ATOM	623	CZ	TYR E	146	98.144	35.925 -10.331	1.00 20.00	6
	ATOM	624	OH	TYR E	146	98.920	34.981 -9.706	1.00 20.00	8
		625	C				40.884 -12.293	1.00 20.00	6
	ATOM			TYR I		94.357			
	ATOM	626	0	TYR I	3 146	94.933	41.963 -12.160	1.00 20.00	8
10	ATOM	627	N	PHE E	3 147	93.326	40.722 -13.110	1.00 20.00	7
	ATOM	628	CA	PHE I	147	92.855	41.832 -13.923	1.00 20.00	6
	ATOM	629	СВ	PHE I		93.823	42.044 -15.092	1.00 20.00	6
	ATOM	630	CG	PHE I	3 147	94.027	40.809 -15.945	1.00 20.00	6
	ATOM	631	CD1	PHE I	3 147	93.049	40.397 -16.850	1.00 20.00	6
15	ATOM	632		PHE I		95.188	40.047 -15.822	1.00 20.00	6
13									
	ATOM	633		PHE I		93.221	39.247 -17.617	1.00 20.00	6
	ATOM	634	CE2	PHE I	3 147	95.372	38.893 -16.585	1.00 20.00	6
	ATOM	635	CZ	PHE E	147	94.388	38.490 -17.485	1.00 20.00	6
	ATOM	636	C	PHE I		91.473	41.566 -14.480	1.00 20.00	6
•									
20	ATOM	637	0	PHE I	3 14/	90.972	40.442 -14.423	1.00 20.00	8
	ATOM	638	N	THR E	3 148	90.865	42.616 -15.021	1.00 20.00	7
	ATOM	639	CA	THR E	148	89.560	42.509 -15.643	1.00 20.00	6
			СВ	THR I			42.889 -14.678	1.00 20.00	
	ATOM	640				88.402			6
	ATOM	641	OG1	THR I	3 148	88.492	44.275 -14.338	1.00 20.00	8
25	ATOM	642	CG2	THR E	3 148	88.460	42.057 -13.403	1.00 20.00	6
	ATOM	643	С	THR E	148	89.532	43.469 -16.821	1.00 20.00	6
				THR I		90.281	44.448 -16.866	1.00 20.00	8
	ATOM	644	0						
	ATOM	645	N	PHE I	3 149	88.685	43.161 -17.791	1.00 20.00	7
	ATOM	646	CA	PHE I	3 149	88.508	44.011 -18.948	1.00 20.00	6
30	ATOM	647	СВ	PHE I		89.750	44.013 -19.864	1.00 20.00	6
50									
	ATOM	648	CG	PHE I		90.133	42.664 -20.419	1.00 20.00	6
	ATOM	649	CD1	PHE I	3 149	89.552	42.182 -21.587	1.00 20.00	6
	ATOM	650	CD2	PHE E	3 149	91.122	41.903 -19.802	1.00 20.00	6
	ATOM	651	CE1	PHE I	149	89.953	40.965 -22.142	1.00 20.00	6
25									
35	ATOM	652		PHE I		91.532	40.681 -20.345	1.00 20.00	6
	ATOM	653	CZ	PHE I	3 149	90.948	40.213 -21.517	1.00 20.00	6
	ATOM	654	С	PHE E	3 149	87.271	43.498 -19.649	1.00 20.00	6
	ATOM	655	0	PHE I	149	86.714	42.474 -19.251	1.00 20.00	8
				GLN H				1.00 20.00	7
4.0	ATOM	656	N			86.812	44.221 -20.657		
40	ATOM	657	CA	GLN E	3 150	85.619	43.807 -21.372	1.00 20.00	6
	MOTA	658	CB	GLN H	150	84.358	44.260 -20.614	1.00 20.00	6
	ATOM	659	CG	GLN E	150	84.302	45.761 -20.289	1.00 20.00	6
				GLN H				1.00 20.00	
	ATOM	660	CD			83.011	46.172 -19.567		6
	MOTA	661	OE I	GLN E	3 150	81.970	46.385 -20.196	1.00 20.00	8
45	ATOM	662	NE2	GLN E	150	83.078	46.273 -18.240	1.00 20.00	7
	ATOM	663	С	GLN H		85.598	44.400 -22.760	1.00 20.00	6
	ATOM	664	0	GLN H		86.281	45.387 -23.033	1.00 20.00	8
	MOTA	665	N	ASP E	3 151	84.846	43.766 -23.649	1.00 20.00	7
	ATOM	666	CA	ASP E	3 151	84.683	44.296 -24.992	1.00 20.00	6
50	ATOM	667	СВ	ASP E		85.160	43.312 -26.074	1.00 20.00	6
50									
	ATOM	668	CG	ASP E		84.558	41.934 -25.939	1.00 20.00	6
	ATOM	669	OD1	ASP I	3 151	83.425	41.812 -25.436	1.00 20.00	8
	ATOM	670	OD2	ASP E	151	85.227	40.963 -26.365	1.00 20.00	8
	ATOM	671	C	ASP I		83.188	44.573 -25.095	1.00 20.00	6
55	ATOM	672	0	ASP I		82.501	44.610 -24.069	1.00 20.00	8
	MOTA	673	N	ASP I	3 152	82.669	44.758 -26.301	1.00 20.00	7
	ATOM	674	CA	ASP E		81.251	45.062 -26.437	1.00 20.00	6
	ATOM	675	СВ	ASP E		80.907	45.346 -27.901	1.00 20.00	6
	ATOM	676	CG	ASP I) I3Z	81.616	46.574 -28.432	1.00 20.00	6

					_	4.50	04 540	45 555 05 666 4 00 00 00
	ATOM	677		ASP :			81.748	47.555 -27.666 1.00 20.00 8
	ATOM	678	OD2	ASP :	В	152	82.030	46.563 -29.613 1.00 20.00 8
	ATOM	679	С	ASP :	В	152	80.285	44.020 -25.888 1.00 20.00 6
	ATOM	680	0	ASP			79.229	44.367 -25.357 1.00 20.00 8
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5	ATOM	681	N	GLU :			80.641	42.747 -25.982 1.00 20.00 7
	ATOM	682	CA	GLU :	В	153	79.727	41.711 -25.521 1.00 20.00 6
	ATOM	683	СВ	GLU :	В	153	79.516	40.685 -26.641 1.00 20.00 6
		684	CG	GLU				41.260 -28.058 1.00 20.00 6
	ATOM						79.577	
	ATOM	685	CD	GLU :	В	153	81.006	41.472 -28.550 1.00 20.00 6
10	ATOM	686	OE1	GLU :	В	153	81.765	40.480 -28.635 1.00 20.00 8
	ATOM	687	OE2	GLU :	R	153	81.374	42.627 -28.854 1.00 20.00 8
	ATOM	688	С	GLU :			80.102	40.960 -24.247 1.00 20.00 6
	ATOM	689	0	GLU :	В	153	79.222	40.473 -23.535 1.00 20.00 8
	ATOM	690	N	LYS	В	154	81.393	40.869 -23.944 1.00 20.00 7
15	ATOM	691	CA	LYS			81.818	40.091 -22.787 1.00 20.00 6
13								
	ATOM	692	СВ	LYS	В	154	82.549	38.830 -23.273 1.00 20.00 6
	ATOM	693	CG	LYS	В	154	81.785	37.978 -24.278 1.00 20.00 6
	ATOM	694	CD	LYS	В	154	82.727	37.028 -25.021 1.00 20.00 6
	ATOM	695	CE	LYS			81.968	36.086 -25.952 1.00 20.00 6
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20	ATOM	696	NZ	LYS			82.894	35.300 -26.826 1.00 20.00 7
	ATOM	697	С	LYS	В	154	82.709	40.767 -21.756 1.00 20.00 6
	ATOM	698	0	LYS	В	154	83.412	41.740 -22.048 1.00 20.00 8
		699	N	LEU			82.677	40.202 -20.551 1.00 20.00 7
	ATOM							
	ATOM	700	CA	LEU			83.501	40.638 -19.428 1.00 20.00 6
25	ATOM	701	CB	LEU :	В	155	82.700	40.651 -18.127 1.00 20.00 6
	ATOM	702	CG	LEU :	В	155	81.451	41.521 -18.004 1.00 20.00 6
	ATOM	703		LEU			80.805	41.273 -16.645 1.00 20.00 6
	ATOM	704	CD2	LEU :	В	155	81.831	42.983 -18.152 1.00 20.00 6
	ATOM	705	С	LEU :	В	155	84.578	39.559 -19.302 1.00 20.00 6
30	ATOM	706	0	LEU :	В	155	84.288	38.379 -19.495 1.00 20.00 8
-	ATOM	707	N	TYR			85.802	39.956 -18.966 1.00 20.00 7
	ATOM	708	CA	TYR	В	156	86.893	38.998 -18.809 1.00 20.00 6
	ATOM	709	СВ	TYR	В	156	87.953	39.189 -19.904 1.00 20.00 6
	ATOM	710	CG	TYR	В	156	87.450	39.053 -21.324 1.00 20.00 6
35		711		TYR			86.688	40.061 -21.920 1.00 20.00 6
33	ATOM							
	ATOM	712	CEI	TYR :			86.233	39.938 -23.235 1.00 20.00 6
	ATOM	713	CD2	TYR	В	156	87.741	37.917 -22.077 1.00 20.00 6
	ATOM	714	CE2	TYR	В	156	87.288	37.782 -23.387 1.00 20.00 6
	ATOM	715	CZ	TYR			86.538	38.794 -23.958 1.00 20.00 6
40								
40	ATOM	716	OH	TYR			86.087	38.656 -25.246 1.00 20.00 8
	ATOM	717	С	TYR	В	156	87.566	39.182 -17.447 1.00 20.00 6
	ATOM	718	0	TYR	В	156	87.977	40.291 -17.110 1.00 20.00 8
	ATOM	719	N	PHE			87.657	38.104 -16.667 1.00 20.00 7
				PHE			88.325	
	ATOM	720	CA					
45	ATOM	721	СВ	PHE	В	157	87.448	37.575 -14.246 1.00 20.00 6
	ATOM	722	CG	PHE	В	157	86.194	38.360 -13.968 1.00 20.00 6
	ATOM	723	CD1	PHE	R	157	85.986	39.614 -14.535 1.00 20.00 6
							85.206	
	ATOM	724		PHE				
	ATOM	725	CE1	PHE	В	157	84.808	40.324 -14.290 1.00 20.00 6
50	ATOM	726	CE2	PHE	В	157	84.025	38.532 -12.893 1.00 20.00 6
	ATOM	727	CZ	PHE			83.829	39.782 -13.470 1.00 20.00 6
	ATOM	728	С	PHE			89.579	37.295 -15.471 1.00 20.00 6
	ATOM	729	0	PHE	В	157	89.492	36.105 -15.765 1.00 20.00 8
	ATOM	730	N	GLY :	В	158	90.742	37.893 -15.231 1.00 20.00 7
55	ATOM	731	CA	GLY :			91.985	37.146 -15.303 1.00 20.00 6
55								
	ATOM	732	С	GLY			92.254	36.512 -13.955 1.00 20.00 6
	ATOM	733	0	GLY :	В	158	92.575	37.211 -12.996 1.00 20.00 8
	ATOM	734	N	LEU :	В	159	92.137	35.191 -13.886 1.00 20.00 7
	ATOM	735	CA	LEU :			92.330	34.466 -12.634 1.00 20.00 6
	111 01.1	, 55	017	110	_		52.550	31.130 12.031 1.00 20.00 0

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91.116 33.580 -12.358 1.00 20.00
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                  CD2 LEU B 159
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	ATOM	796	CA	LEU	В	167	89.651	18.626	-5.168	1.00 20.0) 6
	ATOM	797	СВ	LEU	В	167	89.395	19.269	-3.802	1.00 20.0) 6
	ATOM	798	CG	LEU		167	89.408	18.363	-2.569	1.00 20.0	
_											
5	ATOM	799		LEU		167	90.769	17.703	-2.412	1.00 20.0	
	ATOM	800	CD2	LEU	В	167	89.065	19.193	-1.338	1.00 20.00) 6
	ATOM	801	С	LEU	В	167	88.757	17.394	-5.346	1.00 20.0) 6
				LEU						1.00 20.0	
	ATOM	802	0				89.124	16.283	-4.968		
	ATOM	803	N	LEU	В	168	87.580	17.600	-5.927	1.00 20.0	7
10	ATOM	804	CA	LEU	В	168	86.647	16.500	-6.153	1.00 20.00) 6
	ATOM	805	СВ	LEU	R	168	85.364	17.014	-6.809	1.00 20.0) 6
	ATOM	806	CG	LEU			84.292	15.977	-7.168	1.00 20.0	
	ATOM	807	CD1	LEU	В	168	83.883	15.186	-5.929	1.00 20.0) 6
	ATOM	808	CD2	LEU	В	168	83.083	16.687	-7.756	1.00 20.00) 6
15	ATOM	809	С	LEU			87.290	15.440	-7.046	1.00 20.00	
13											
	ATOM	810	0	LEU			87.091	14.243	-6.845	1.00 20.0	
	ATOM	811	N	LYS	В	169	88.068	15.888	-8.027	1.00 20.0	7
	ATOM	812	CA	LYS	В	169	88.727	14.967	-8.941	1.00 20.0) 6
	ATOM	813	СВ	LYS			89.610	15.729	-9.930	1.00 20.0	
20											
20	ATOM	814	CG	LYS			90.379		-10.882	1.00 20.0	
	ATOM	815	CD	LYS	В	169	91.226	15.603	-11.877	1.00 20.00) 6
	ATOM	816	CE	LYS	В	169	92.373	16.328	-11.192	1.00 20.00) 6
		817	ΝZ	LYS			93.253		-12.173	1.00 20.0	
	ATOM										
	ATOM	818	С	LYS			89.574	13.949	-8.193	1.00 20.0	
25	ATOM	819	0	LYS	В	169	89.543	12.758	-8.504	1.00 20.00	8 (
	ATOM	820	N	TYR	В	170	90.334	14.417	-7.207	1.00 20.0	7
	ATOM	821	CA	TYR			91.197	13.527	-6.441	1.00 20.00	
	ATOM	822	СВ	TYR	В	170	92.243	14.346	-5.682	1.00 20.0) 6
	ATOM	823	CG	TYR	В	170	93.217	15.010	-6.624	1.00 20.0) 6
30	ATOM	824	CD1	TYR	В	170	94.347	14.331	-7.085	1.00 20.00) 6
-	ATOM	825		TYR		170	95.195	14.900	-8.036	1.00 20.0	
	ATOM	826	CD2	TYR	В	170	92.963	16.282	-7.133	1.00 20.0) 6
	ATOM	827	CE2	TYR	В	170	93.801	16.861	-8.083	1.00 20.00) 6
	ATOM	828	CZ	TYR	В	170	94.913	16.164	-8.532	1.00 20.0) 6
35		829	OH	TYR		170				1.00 20.0	
33	ATOM						95.727	16.727	-9.493		
	ATOM	830	С	TYR	В	170	90.419	12.622	-5.499	1.00 20.0	
	ATOM	831	0	TYR	В	170	90.834	11.494	-5.233	1.00 20.00	8 (
	ATOM	832	N	ILE	В	171	89.287	13.098	-4.993	1.00 20.00	7
	ATOM	833	CA	ILE			88.488	12.262	-4.112	1.00 20.00	
40											
40	ATOM	834	СВ	ILE			87.278	13.028	-3.538	1.00 20.0	
	ATOM	835	CG2	ILE	В	171	86.367	12.065	-2.791	1.00 20.0) 6
	ATOM	836	CG1	ILE	В	171	87.764	14.141	-2.603	1.00 20.00) 6
	ATOM	837		ILE	В	171	86.652	14.990	-2.019	1.00 20.00	
	ATOM	838	C	ILE			87.994	11.066	-4.931	1.00 20.0	
45	ATOM	839	0	ILE	В	171	88.030	9.925	-4.468	1.00 20.0	
	ATOM	840	N	ARG	В	172	87.550	11.331	-6.156	1.00 20.00	7
	ATOM	841	CA	ARG			87.061	10.273	-7.031	1.00 20.00	
									-8.259	1.00 20.00	
	ATOM	842	СВ	ARG			86.359	10.861			
	ATOM	843	CG	ARG	В	172	85.094	11.658	-7.963	1.00 20.0) 6
50	ATOM	844	CD	ARG	В	172	84.352	11.981	-9.259	1.00 20.00) 6
	ATOM	845	NE	ARG	В	172	83.187	12.843	-9.063	1.00 20.00	
	ATOM	846	CZ	ARG			82.192	12.589	-8.217	1.00 20.0	
	ATOM	847	NH1	ARG	В	172	82.209	11.491	-7.469	1.00 20.0	
	ATOM	848	NH2	ARG	В	172	81.168	13.428	-8.127	1.00 20.00	7
55	ATOM	849	С	ARG			88.202	9.378	-7.497	1.00 20.0	
55											
	ATOM	850	0	ARG			88.050	8.160	-7.587	1.00 20.00	
	ATOM	851	N	LYS	В	173	89.348	9.985	-7.783	1.00 20.0	
	ATOM	852	CA	LYS	В	173	90.509	9.244	-8.256	1.00 20.00) 6
	ATOM	853	СВ	LYS			91.647	10.206	-8.603	1.00 20.00	
	111 011	555	010	1110	יב	1,0) I • OI /	-0.200	0.003	1.00 20.0	, 0

	ATOM	854	CG	LYS	В	173	92.930	9.511	-9.045	1.00 20.0	0 6
	ATOM	855	CD	LYS	В	173	94.081	10.496	-9.222	1.00 20.0	0 6
	ATOM	856	CE	LYS	В	173	93.862	11.432	-10.406	1.00 20.0	0 6
	ATOM	857	NZ	LYS	В	173	93.858	10.711	-11.715	1.00 20.0	0 7
5	MOTA	858	С	LYS	В	173	91.025	8.191	-7.280	1.00 20.0	0 6
	MOTA	859	0	LYS	В	173	91.274	7.055	-7.674	1.00 20.0	0 8
	MOTA	860	N	ILE	В	174	91.192	8.554	-6.012	1.00 20.0	0 7
	ATOM	861	CA	ILE	В	174	91.710	7.593	-5.042	1.00 20.0	0 6
	ATOM	862	СВ	ILE	В	174	92.884	8.191	-4.223	1.00 20.0	0 6
10	ATOM	863	CG2	ILE	В	174	93.970	8.701	-5.166	1.00 20.0	0 6
	ATOM	864	CG1	ILE	В	174	92.394	9.337	-3.343	1.00 20.0	0 6
	ATOM	865	CD1	ILE	В	174	93.480	9.916	-2.457	1.00 20.0	0 6
	ATOM	866	С	ILE	В	174	90.674	7.030	-4.074	1.00 20.0	0 6
	ATOM	867	0	ILE	В	174	91.025	6.296	-3.151	1.00 20.0	0 8
15	ATOM	868	N	GLY	В	175	89.405	7.367	-4.283	1.00 20.0	0 7
	ATOM	869	CA	GLY	В	175	88.359	6.855	-3.413	1.00 20.0	0 6
	ATOM	870	С	GLY	В	175	88.160	7.650	-2.138	1.00 20.0	0 6
	ATOM	871	0	GLY	В	175	87.083	8.198	-1.905	1.00 20.0	0 8
	ATOM	872	N	SER	В	176	89.192	7.701	-1.304	1.00 20.0	0 7
20	ATOM	873	CA	SER	В	176	89.140	8.447	-0.053	1.00 20.0	0 6
	ATOM	874	СВ	SER	В	176	88.395	7.653	1.026	1.00 20.0	0 6
	ATOM	875	OG	SER	В	176	89.150	6.543	1.472	1.00 20.0	0 8
	ATOM	876	С	SER	В	176	90.565	8.742	0.401	1.00 20.0	0 6
	ATOM	877	0	SER	В	176	91.506	8.049	0.009	1.00 20.0	0 8
25	ATOM	878	N	PHE	В	177	90.718	9.769	1.228	1.00 20.0	0 7
	ATOM	879	CA	PHE	В	177	92.029	10.184	1.722	1.00 20.0	0 6
	ATOM	880	СВ	PHE	В	177	92.028	11.694	1.990	1.00 20.0	0 6
	ATOM	881	CG	PHE	В	177	92.002	12.546	0.747	1.00 20.0	0 6
	ATOM	882	CD1	PHE	В	177	91.484	12.060	-0.449	1.00 20.0	0 6
30	ATOM	883	CD2	PHE	В	177	92.481	13.855	0.787	1.00 20.0	0 6
	ATOM	884	CE1	PHE	В	177	91.443	12.860	-1.585	1.00 20.0	
	ATOM	885	CE2	PHE	В	177	92.444	14.665	-0.343	1.00 20.0	
	ATOM	886	CZ	PHE	В	177	91.925	14.168	-1.532	1.00 20.0	0 6
	ATOM	887	С	PHE	В	177	92.427	9.475	3.009	1.00 20.0	
35	ATOM	888	0	PHE	В	177	91.582	9.223	3.872	1.00 20.0	00 8
	ATOM	889	N	ASP		178	93.711	9.152	3.147	1.00 20.0	0 7
	ATOM	890	CA	ASP	В	178	94.155	8.529	4.385	1.00 20.0	
	ATOM	891	СВ	ASP		178	95.581	7.972	4.267	1.00 20.0	
	ATOM	892	CG	ASP	В	178	96.594	9.018	3.845	1.00 20.0	
40	ATOM	893	OD1	ASP	В	178	96.392	10.214	4.139	1.00 20.0	
	ATOM	894		ASP		178	97.612	8.634	3.230	1.00 20.0	00 8
	ATOM	895	С	ASP	В	178	94.092	9.640	5.436	1.00 20.0	0 6
	ATOM	896	0	ASP	В	178	93.736	10.778	5.117	1.00 20.0	0 8
	ATOM	897	N	GLU	В	179	94.443	9.324	6.677	1.00 20.0	
45	ATOM	898	CA	GLU			94.380	10.311	7.744	1.00 20.0	
	ATOM	899	СВ	GLU	В	179	94.623	9.637	9.096	1.00 20.0	0 6
	ATOM	900	CG	GLU	В	179	94.747	10.611	10.255	1.00 20.0	
	ATOM	901	CD	GLU	В	179	94.331	9.994	11.574	1.00 20.0	
	ATOM	902	OE1	GLU			94.589	8.789	11.770	1.00 20.0	
50	ATOM	903	OE2	GLU	В	179	93.753	10.717	12.416	1.00 20.0	
	ATOM	904	С	GLU			95.320	11.501	7.575	1.00 20.0	
	ATOM	905	0	GLU	В	179	94.948	12.636	7.881	1.00 20.0	
	ATOM	906	N	THR			96.528	11.246	7.086	1.00 20.0	
	ATOM	907	CA	THR			97.509	12.308	6.886	1.00 20.0	
55	ATOM	908	СВ	THR			98.866	11.720	6.445	1.00 20.0	
	ATOM	909		THR			99.349	10.842	7.466	1.00 20.0	
	ATOM	910		THR			99.888	12.825	6.213	1.00 20.0	
	ATOM	911	С	THR			97.040	13.331	5.849	1.00 20.0	
	ATOM	912	0	THR			97.136	14.542	6.069	1.00 20.0	

	ATOM	913	N	CYS	В	181	96.534	12.845	4.721	1.00	20.00	7
	ATOM	914	CA	CYS	В	181	96.057	13.733	3.666	1.00	20.00	6
	ATOM	915	СВ	CYS	В	181	95.836	12.945	2.375	1.00	20.00	6
				CYS			97.372				20.00	
_	ATOM	916	SG					12.255	1.685			16
5	MOTA	917	С	CYS	В	181	94.775	14.449	4.079	1.00	20.00	6
	ATOM	918	0	CYS	В	181	94.570	15.615	3.733	1.00	20.00	8
	ATOM	919	N	THR	В	182	93.914	13.755	4.820	1.00	20.00	7
				THR				14.356			20.00	6
	ATOM	920	CA				92.669		5.286			
	ATOM	921	СВ	THR	В	182	91.812	13.354	6.103	1.00	20.00	6
10	ATOM	922	OG1	THR	В	182	91.372	12.283	5.259	1.00	20.00	8
	ATOM	923	CG2	THR	В	182	90.600	14.054	6.690	1.00	20.00	6
			C	THR								6
	ATOM	924					93.014	15.535	6.196		20.00	
	MOTA	925	0	THR	В	182	92.515	16.649	6.019	1.00	20.00	8
	ATOM	926	N	ARG	В	183	93.873	15.273	7.175	1.00	20.00	7
15	ATOM	927	CA	ARG	В	183	94.299	16.293	8.121	1.00	20.00	6
15		928	СВ	ARG				15.707			20.00	6
	ATOM						95.311		9.109			
	ATOM	929	CG	ARG	В	183	95.957	16.744	10.012	1.00	20.00	6
	ATOM	930	CD	ARG	В	183	96.886	16.116	11.050	1.00	20.00	6
	ATOM	931	NE	ARG	В	183	96.167	15.220	11.949	1.00	20.00	7
20	ATOM	932	CZ	ARG			96.098	13.900	11.804		20.00	6
20												
	ATOM	933		ARG			96.717	13.306	10.791		20.00	7
	MOTA	934	NH2	ARG	В	183	95.389	13.176	12.664	1.00	20.00	7
	ATOM	935	С	ARG	В	183	94.923	17.505	7.427	1.00	20.00	6
	ATOM	936	0	ARG	R	183	94.545	18.646	7.698		20.00	8
25												
25	ATOM	937	N	PHE		184	95.877	17.264	6.534		20.00	7
	ATOM	938	CA	PHE	В	184	96.539	18.367	5.847	1.00	20.00	6
	ATOM	939	СВ	PHE	В	184	97.610	17.847	4.889	1.00	20.00	6
	ATOM	940	CG	PHE	В	184	98.387	18.943	4.223	1.00	20.00	6
	ATOM	941		PHE			99.451	19.555	4.879		20.00	6
20												
30	ATOM	942		PHE		184	98.009	19.415	2.975		20.00	6
	MOTA	943	CE1	PHE	В	184	100.125	20.627	4.301	1.00	20.00	6
	ATOM	944	CE2	PHE	В	184	98.676	20.491	2.388	1.00	20.00	6
	ATOM	945	CZ	PHE			99.735	21.097	3.053		20.00	6
	ATOM	946	С	PHE		184	95.580	19.267	5.066		20.00	6
35	ATOM	947	0	PHE	В	184	95.567	20.481	5.255	1.00	20.00	8
	ATOM	948	N	TYR	В	185	94.784	18.679	4.181	1.00	20.00	7
	ATOM	949	CA	TYR	В	185	93.854	19.471	3.390	1.00	20.00	6
	ATOM	950	СВ	TYR			93.305	18.634	2.236		20.00	6
	ATOM	951	CG	TYR		185	94.337	18.504	1.140		20.00	6
40	MOTA	952	CD1	TYR	В	185	94.611	19.580	0.293	1.00	20.00	6
	ATOM	953	CE1	TYR	В	185	95.637	19.516	-0.643	1.00	20.00	6
	ATOM	954	CD2	TYR	R	185	95.118	17.352	1.017	1 00	20.00	6
	ATOM	955		TYR			96.152	17.282	0.081		20.00	6
	ATOM	956	CZ	TYR			96.405	18.367	-0.742	1.00	20.00	6
45	ATOM	957	OH	TYR	В	185	97.436	18.314	-1.657	1.00	20.00	8
	ATOM	958	С	TYR	В	185	92.738	20.098	4.208	1.00	20.00	6
	ATOM	959	0	TYR			92.286	21.195	3.891		20.00	8
	ATOM	960	N	THR			92.303	19.422	5.267		20.00	7
	MOTA	961	CA	THR	В	186	91.265	19.987	6.122	1.00	20.00	6
50	ATOM	962	СВ	THR	В	186	90.799	18.996	7.219	1.00	20.00	6
	ATOM	963	0G1	THR			90.193	17.846	6.606	1 00	20.00	8
				THR			89.774					
	ATOM	964						19.671	8.144		20.00	6
	ATOM	965	С	THR			91.858	21.218	6.805		20.00	6
	ATOM	966	0	THR	В	186	91.188	22.242	6.948	1.00	20.00	8
55	ATOM	967	N	ALA			93.120	21.115	7.222		20.00	7
	ATOM	968	CA	ALA			93.787	22.234	7.882		20.00	6
	ATOM	969	СВ	ALA			95.184	21.817	8.349		20.00	6
	ATOM	970	С	ALA	В	187	93.879	23.449	6.946	1.00	20.00	6
	ATOM	971	0	ALA	В	187	93.654	24.585	7.372	1.00	20.00	8

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	MOTA	972	N	GLU			94.205	23.222	5.674	1.00 20.00	7
	ATOM	973	CA	GLU	В	188	94.292	24.343	4.740	1.00 20.00	6
	ATOM	974	СВ	GLU	В	188	94.843	23.898	3.376	1.00 20.00	6
	ATOM	975	CG	GLU		188	96.285	23.391	3.407	1.00 20.00	6
_											
5	ATOM	976	CD	GLU		188	97.030	23.639	2.104	1.00 20.00	6
	ATOM	977	OE1	GLU	В	188	96.407	23.537	1.024	1.00 20.00	8
	ATOM	978	OE2	GLU	В	188	98.247	23.932	2.156	1.00 20.00	8
		979	C	GLU		188			4.561	1.00 20.00	6
	MOTA						92.912	24.977			
	ATOM	980	0	GLU	В	188	92.782	26.196	4.533	1.00 20.00	8
10	ATOM	981	N	ILE	В	189	91.875	24.152	4.451	1.00 20.00	7
	ATOM	982	CA	ILE	В	189	90.530	24.693	4.284	1.00 20.00	6
	MOTA	983	СВ	ILE			89.495	23.566	4.064	1.00 20.00	6
	ATOM	984	CG2	ILE	В	189	88.094	24.157	3.947	1.00 20.00	6
	ATOM	985	CG1	ILE	В	189	89.855	22.773	2.796	1.00 20.00	6
15	ATOM	986	CD1	ILE	В	189	89.058	21.488	2.616	1.00 20.00	6
13											
	ATOM	987	С	ILE			90.152	25.517	5.519	1.00 20.00	6
	ATOM	988	0	ILE	В	189	89.634	26.630	5.396	1.00 20.00	8
	ATOM	989	N	VAL	В	190	90.412	24.971	6.707	1.00 20.00	7
	ATOM	990	CA	VAL	R	190	90.116	25.674	7.957	1.00 20.00	6
20							90.557		9.186		
20	ATOM	991	СВ	VAL				24.842		1.00 20.00	6
	ATOM	992	CG1	VAL	В	190	90.540	25.717	10.451	1.00 20.00	6
	ATOM	993	CG2	VAL	В	190	89.643	23.641	9.358	1.00 20.00	6
	ATOM	994	С	VAL			90.865	27.012	7.984	1.00 20.00	6
		995		VAL							
	ATOM		0				90.311	28.039	8.375	1.00 20.00	8
25	ATOM	996	N	SER	В	191	92.125	26.997	7.557	1.00 20.00	7
	ATOM	997	CA	SER	В	191	92.934	28.218	7.546	1.00 20.00	6
	ATOM	998	СВ	SER	В	191	94.378	27.888	7.166	1.00 20.00	6
		999	OG	SER			95.220	29.007			8
	ATOM								7.363	1.00 20.00	
	ATOM	1000	С	SER	В	191	92.361	29.240	6.566	1.00 20.00	6
30	ATOM	1001	0	SER	В	191	92.351	30.444	6.838	1.00 20.00	8
	ATOM	1002	N	ALA	В	192	91.882	28.754	5.425	1.00 20.00	7
		1003		ALA			91.306	29.634	4.417	1.00 20.00	
	ATOM		CA								6
	ATOM	1004	СВ	ALA	В	192	91.006	28.850	3.141	1.00 20.00	6
	ATOM	1005	С	ALA	В	192	90.029	30.256	4.970	1.00 20.00	6
35	ATOM	1006	0	ALA	В	192	89.799	31.458	4.822	1.00 20.00	8
	ATOM	1007	N	LEU			89.203	29.439	5.621	1.00 20.00	7
	ATOM	1008	CA	LEU			87.957	29.941	6.192	1.00 20.00	6
	MOTA	1009	CB	LEU	В	193	87.101	28.783	6.725	1.00 20.00	6
	ATOM	1010	CG	LEU	В	193	86.447	27.898	5.650	1.00 20.00	6
40	ATOM	1011	CD1	LEU			85.645	26.771	6.315	1.00 20.00	6
10		1012		LEU			85.530				
	MOTA							28.752	4.780	1.00 20.00	6
	ATOM	1013	С	LEU	В	193	88.215	30.959	7.299	1.00 20.00	6
	ATOM	1014	0	LEU	В	193	87.474	31.935	7.435	1.00 20.00	8
	ATOM	1015	N	GLU	В	194	89.254	30.738	8.100	1.00 20.00	7
45	ATOM	1016	CA	GLU			89.562	31.699	9.157	1.00 20.00	6
43											
	MOTA	1017	СВ	GLU			90.773	31.257	9.982	1.00 20.00	6
	ATOM	1018	CG	GLU	В	194	91.288	32.353	10.914	1.00 20.00	6
	ATOM	1019	CD	GLU	В	194	92.381	31.878	11.855	1.00 20.00	6
	ATOM	1020		GLU			93.246	31.090	11.420	1.00 20.00	8
50											
50	ATOM	1021	OE2	GLU			92.376	32.312	13.031	1.00 20.00	8
	ATOM	1022	С	GLU	В	194	89.847	33.053	8.511	1.00 20.00	6
	ATOM	1023	0	GLU	В	194	89.375	34.083	8.972	1.00 20.00	8
	ATOM	1024	N	TYR			90.608	33.046	7.426	1.00 20.00	7
_	MOTA	1025	CA	TYR			90.928	34.294	6.743	1.00 20.00	6
55	MOTA	1026	СВ	TYR	В	195	91.919	34.043	5.613	1.00 20.00	6
	ATOM	1027	CG	TYR	В	195	92.193	35.271	4.774	1.00 20.00	6
	ATOM	1028		TYR			93.098	36.244	5.202	1.00 20.00	6
	ATOM	1029		TYR			93.356	37.382	4.429	1.00 20.00	6
	ATOM	1030	CD2	TYR	В	195	91.545	35.461	3.553	1.00 20.00	6

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	ATOM	1031		TYR			91.794	36.591	2.775	1.00 20.00	6
	ATOM	1032	CZ	TYR			92.701	37.545	3.219	1.00 20.00	6
	ATOM	1033	OH	TYR	В	195	92.956	38.656	2.450	1.00 20.00	8
	ATOM	1034	С	TYR	В	195	89.668	34.923	6.160	1.00 20.00	6
5	ATOM	1035	0	TYR			89.409	36.117	6.328	1.00 20.00	8
5		1036		LEU			88.885			1.00 20.00	7
	ATOM		N					34.103	5.472		
	MOTA	1037	CA	LEU	В	196	87.664	34.576	4.845	1.00 20.00	6
	ATOM	1038	CB	LEU	В	196	86.972	33.426	4.107	1.00 20.00	6
	ATOM	1039	CG	LEU	В	196	85.933	33.824	3.060	1.00 20.00	6
10	ATOM	1040	CD1	LEU			86.602	34.659	1.966	1.00 20.00	6
	ATOM	1041		LEU			85.305	32.568	2.463	1.00 20.00	6
	ATOM	1042	С	LEU			86.731	35.161	5.888	1.00 20.00	6
	ATOM	1043	0	LEU			86.299	36.308	5.774	1.00 20.00	8
	ATOM	1044	N	HIS	В	197	86.431	34.378	6.917	1.00 20.00	7
15	ATOM	1045	CA	HIS	В	197	85.533	34.840	7.967	1.00 20.00	6
	ATOM	1046	СВ	HIS	В	197	85.241	33.697	8.942	1.00 20.00	6
	ATOM	1047	CG	HIS			84.377	32.622	8.356	1.00 20.00	6
	ATOM	1048		HIS			83.734	32.550	7.163	1.00 20.00	6
	MOTA	1049		HIS			84.083	31.452	9.022	1.00 20.00	7
20	ATOM	1050	CE1	HIS	В	197	83.296	30.704	8.264	1.00 20.00	6
	ATOM	1051	NE2	HIS	В	197	83.071	31.346	7.132	1.00 20.00	7
	ATOM	1052	С	HIS	В	197	86.080	36.060	8.697	1.00 20.00	6
		1053	0	HIS			85.314	36.919	9.146	1.00 20.00	8
	ATOM										
	ATOM	1054	N	GLY			87.404	36.143	8.804	1.00 20.00	7
25	ATOM	1055	CA	GLY			88.009	37.285	9.464	1.00 20.00	6
	ATOM	1056	С	GLY	В	198	87.687	38.580	8.737	1.00 20.00	6
	ATOM	1057	0	GLY	В	198	87.784	39.661	9.311	1.00 20.00	8
	ATOM	1058	N	LYS	В	199	87.308	38.475	7.466	1.00 20.00	7
	ATOM	1059	CA	LYS			86.959	39.652	6.674	1.00 20.00	6
20											
30	ATOM	1060	СВ	LYS			87.577	39.573	5.279	1.00 20.00	6
	ATOM	1061	CG	LYS			89.082	39.736	5.258	1.00 20.00	6
	ATOM	1062	CD	LYS	В	199	89.574	39.919	3.833	1.00 20.00	6
	ATOM	1063	CE	LYS	В	199	91.054	40.243	3.807	1.00 20.00	6
	ATOM	1064	NΖ	LYS	В	199	91.398	41.382	4.706	1.00 20.00	7
35	ATOM	1065	C	LYS		199	85.451	39.804	6.539	1.00 20.00	6
33											
	ATOM	1066	0	LYS		199	84.972	40.556	5.693	1.00 20.00	8
	ATOM	1067	N	GLY			84.707	39.079	7.368	1.00 20.00	7
	ATOM	1068	$^{\rm CA}$	$\operatorname{GL} Y$	В	200	83.258	39.158	7.328	1.00 20.00	6
	ATOM	1069	С	GLY	В	200	82.646	38.660	6.032	1.00 20.00	6
40	ATOM	1070	0	GLY	В	200	81.644	39.198	5.564	1.00 20.00	8
	ATOM	1071	N	ILE			83.243	37.630	5.445	1.00 20.00	7
	ATOM	1072	CA	ILE			82.726		4.205	1.00 20.00	6
		1072		ILE							
	ATOM		СВ				83.775	37.140	3.080	1.00 20.00	6
	ATOM	1074		ILE			83.257	36.413	1.841	1.00 20.00	6
45	ATOM	1075	CG1	ILE	В	201	84.109	38.599	2.761	1.00 20.00	6
	ATOM	1076	CD1	ILE	В	201	85.330	38.758	1.870	1.00 20.00	6
	ATOM	1077	С	ILE	В	201	82.329	35.623	4.395	1.00 20.00	6
	ATOM	1078	0	ILE			83.094	34.826	4.942	1.00 20.00	8
	ATOM	1079	N	ILE			81.125	35.291	3.940	1.00 20.00	7
50											
50	ATOM	1080	CA	ILE			80.592	33.936	4.016	1.00 20.00	6
	ATOM	1081	СВ	ILE			79.119	33.953	4.481	1.00 20.00	6
	ATOM	1082	CG2	ILE	В	202	78.583	32.522	4.595	1.00 20.00	6
	ATOM	1083	CG1	ILE	В	202	79.008	34.675	5.825	1.00 20.00	6
	ATOM	1084		ILE			77.576	34.865	6.294	1.00 20.00	6
55	ATOM	1085	C	ILE			80.644	33.393	2.589	1.00 20.00	6
55											
	ATOM	1086	0	ILE			80.182	34.056	1.663	1.00 20.00	8
	ATOM	1087	N	HIS			81.204	32.204	2.395	1.00 20.00	7
	ATOM	1088	CA	HIS	В	203	81.279	31.652	1.044	1.00 20.00	6
	ATOM	1089	СВ	HIS	В	203	82.258	30.480	0.999	1.00 20.00	6

	ATOM	1090	CG	HIS	R	203	82.478	29.942	-0.380	1.00 20.00	6
	ATOM	1091		HIS			81.646	29.282	-1.220	1.00 20.00	6
	ATOM	1092		HIS			83.659	30.116	-1.069	1.00 20.00	7
	ATOM	1092		HIS			83.545	29.588	-2.275	1.00 20.00	6
-											
5	ATOM	1094		HIS			82.333	29.076	-2.392	1.00 20.00	7
	ATOM	1095	С	HIS			79.896	31.211	0.530	1.00 20.00	6
	ATOM	1096	0	HIS			79.508	31.546	-0.593	1.00 20.00	8
	ATOM	1097	N	ARG			79.168	30.458	1.357	1.00 20.00	7
	ATOM	1098	CA	ARG			77.819	29.969	1.039	1.00 20.00	6
10	ATOM	1099	СВ	ARG	В	204	76.916	31.117	0.583	1.00 20.00	6
	ATOM	1100	CG	ARG	В	204	76.601	32.120	1.675	1.00 20.00	6
	ATOM	1101	CD	ARG	В	204	75.316	32.878	1.377	1.00 20.00	6
	MOTA	1102	NE	ARG	В	204	75.376	33.616	0.119	1.00 20.00	7
	ATOM	1103	CZ	ARG	В	204	74.423	34.443	-0.303	1.00 20.00	6
15	ATOM	1104	NH1	ARG			73.336	34.636	0.436	1.00 20.00	7
	ATOM	1105		ARG			74.555	35.084	-1.457	1.00 20.00	7
	ATOM	1106	С	ARG			77.700	28.829	0.030	1.00 20.00	6
	ATOM	1107	0	ARG			76.611	28.300	-0.177	1.00 20.00	8
	ATOM	1107	N	ASP			78.792	28.456	-0.620	1.00 20.00	7
20		1100		ASP			78.718			1.00 20.00	6
20	ATOM		CA					27.342	-1.550		
	ATOM	1110	CB	ASP			78.380	27.829	-2.961	1.00 20.00	6
	ATOM	1111	CG	ASP			77.941	26.694	-3.867	1.00 20.00	6
	ATOM	1112		ASP			77.544	25.638	-3.330	1.00 20.00	8
	ATOM	1113		ASP			77.982	26.853	-5.104	1.00 20.00	8
25	ATOM	1114	С	ASP			80.019	26.560	-1.547	1.00 20.00	6
	ATOM	1115	0	ASP	В	205	80.508	26.122	-2.588	1.00 20.00	8
	MOTA	1116	N	LEU	В	206	80.573	26.375	-0.354	1.00 20.00	7
	MOTA	1117	CA	LEU	В	206	81.819	25.652	-0.208	1.00 20.00	6
	ATOM	1118	СВ	LEU	В	206	82.361	25.826	1.212	1.00 20.00	6
30	ATOM	1119	CG	LEU	В	206	83.764	25.271	1.471	1.00 20.00	6
	ATOM	1120	CD1	LEU	В	206	84.765	25.969	0.561	1.00 20.00	6
	ATOM	1121		LEU			84.135	25.477	2.933	1.00 20.00	6
	ATOM	1122	С	LEU			81.609	24.174	-0.514	1.00 20.00	6
	ATOM	1123	0	LEU			80.691	23.549	0.011	1.00 20.00	8
35	ATOM	1124	N	LYS			82.461	23.628	-1.375	1.00 20.00	7
	ATOM	1125	CA	LYS			82.379	22.223	-1.765	1.00 20.00	6
	ATOM	1126	CB	LYS			81.160	22.000	-2.679	1.00 20.00	6
	ATOM	1127	CG	LYS			81.130	22.913	-3.893	1.00 20.00	6
		1128	CD	LYS			79.876	22.720	-4.736	1.00 20.00	6
40	ATOM							23.797	-5.813		
40	ATOM	1129	CE	LYS			79.788 78.695			1.00 20.00	6 7
	ATOM	1130	ΝZ	LYS				23.557	-6.791	1.00 20.00	
	ATOM	1131	С	LYS			83.657		-2.487	1.00 20.00	6
	ATOM	1132	0	LYS			84.416	22.656	-2.960	1.00 20.00	8
	MOTA	1133	N	PRO			83.916	20.494	-2.582	1.00 20.00	7
45	ATOM	1134	CD	PRO			83.153	19.378	-1.993	1.00 20.00	6
	MOTA	1135	CA	PRO			85.122	20.005	-3.259	1.00 20.00	6
	MOTA	1136	CB	PRO	В	208	84.922	18.494	-3.267	1.00 20.00	6
	MOTA	1137	CG	PRO	В	208	84.174	18.256	-1.984	1.00 20.00	6
	ATOM	1138	С	PRO	В	208	85.303	20.574	-4.666	1.00 20.00	6
50	ATOM	1139	0	PRO	В	208	86.431	20.752	-5.124	1.00 20.00	8
	ATOM	1140	N	GLU	В	209	84.197	20.859	-5.347	1.00 20.00	7
	ATOM	1141	CA	GLU			84.243	21.410	-6.705	1.00 20.00	6
	ATOM	1142	СВ	GLU			82.836	21.424	-7.317	1.00 20.00	6
	ATOM	1143	CG	GLU			82.755	22.081	-8.690	1.00 20.00	6
55	ATOM	1144	CD	GLU			81.323	22.296	-9.159	1.00 20.00	6
55	ATOM	1145		GLU			80.587	21.299	-9.322	1.00 20.00	8
				GLU			80.933			1.00 20.00	
	ATOM	1146						23.465	-9.364		8
	ATOM	1147	C	GLU			84.810	22.836	-6.716	1.00 20.00	6
	ATOM	1148	0	GLU	В	209	85.409	23.269	-7.705	1.00 20.00	8

	MOTA	1149	N	ASN	В	210	84.604	23.549	-5.612	1.00 20.00	7
	ATOM	1150	CA	ASN	В	210	85.051	24.932	-5.439	1.00 20.00	6
	ATOM	1151	СВ	ASN	В	210	84.033	25.695	-4.588	1.00 20.00	6
		1152	CG							1.00 20.00	6
_	MOTA			ASN			82.851	26.170	-5.396		
5	MOTA	1153	OD1	ASN	В	210	81.807	26.520	-4.846	1.00 20.00	8
	ATOM	1154	ND2	ASN	В	210	83.010	26.194	-6.717	1.00 20.00	7
	ATOM	1155	С	ASN	В	210	86.427	25.070	-4.797	1.00 20.00	6
		1156								1.00 20.00	8
	ATOM		0	ASN			86.937	26.181	-4.641		
	ATOM	1157	N	ILE	В	211	87.016	23.948	-4.406	1.00 20.00	7
10	ATOM	1158	CA	ILE	В	211	88.331	23.958	-3.790	1.00 20.00	6
	ATOM	1159	СВ	TLE	В	211	88.336	23.090	-2.521	1.00 20.00	6
	ATOM	1160		ILE			89.732	23.025	-1.925	1.00 20.00	6
	ATOM	1161		ILE			87.350	23.682	-1.510	1.00 20.00	6
	ATOM	1162	CD1	ILE	В	211	87.121	22.832	-0.285	1.00 20.00	6
15	ATOM	1163	С	ILE	В	211	89.307	23.414	-4.816	1.00 20.00	6
	ATOM	1164	0	ILE			89.475	22.199	-4.949	1.00 20.00	8
	ATOM	1165	N	LEU			89.938	24.319	-5.558	1.00 20.00	7
	ATOM	1166	CA	LEU	В	212	90.875	23.918	-6.601	1.00 20.00	6
	ATOM	1167	СВ	LEU	В	212	90.966	25.012	-7.673	1.00 20.00	6
20	ATOM	1168	CG	LEU	В	212	89.630	25.510	-8.235	1.00 20.00	6
	ATOM	1169		LEU			89.896	26.462	-9.390	1.00 20.00	6
	ATOM	1170	CD2	LEU			88.781	24.331	-8.709	1.00 20.00	6
	MOTA	1171	С	LEU	В	212	92.254	23.628	-6.038	1.00 20.00	6
	ATOM	1172	0	LEU	В	212	92.537	23.923	-4.873	1.00 20.00	8
25	ATOM	1173	N	LEU	В	213	93.114	23.053	-6.875	1.00 20.00	7
	ATOM	1174	CA	LEU			94.472	22.714	-6.472	1.00 20.00	6
	ATOM	1175	СВ	LEU	В	213	94.609	21.192	-6.388	1.00 20.00	6
	ATOM	1176	CG	LEU	В	213	93.775	20.526	-5.292	1.00 20.00	6
	ATOM	1177	CD1	LEU	В	213	93.737	19.035	-5.508	1.00 20.00	6
30	ATOM	1178		LEU			94.374	20.852	-3.935	1.00 20.00	6
50		1179	C					23.277		1.00 20.00	6
	ATOM			LEU			95.503		-7.449		
	ATOM	1180	0	LEU			95.422	23.033	-8.657	1.00 20.00	8
	MOTA	1181	N	ASN	В	214	96.470	24.036	-6.940	1.00 20.00	7
	ATOM	1182	CA	ASN	В	214	97.488	24.585	-7.826	1.00 20.00	6
35	ATOM	1183	СВ	ASN			98.198	25.792	-7.201	1.00 20.00	6
55			CG	ASN						1.00 20.00	
	ATOM	1184					98.938	25.448	-5.927		6
	ATOM	1185		ASN			99.267	24.288	-5.669	1.00 20.00	8
	MOTA	1186	ND2	ASN	В	214	99.224	26.469	-5.123	1.00 20.00	7
	ATOM	1187	С	ASN	В	214	98.508	23.515	-8.182	1.00 20.00	6
40	ATOM	1188	0	ASN			98.420	22.372	-7.725	1.00 20.00	8
10		1189	N	GLU			99.482	23.894	-8.996	1.00 20.00	7
	ATOM										
	ATOM	1190	CA	GLU			100.514	22.965	-9.430	1.00 20.00	6
	MOTA	1191	СВ	GLU	В	215	101.491	23.687	-10.362	1.00 20.00	6
	ATOM	1192	CG	GLU	В	215	102.544	22.788	-10.979	1.00 20.00	6
45	ATOM	1193	CD	GLU			103.323		-12.080	1.00 20.00	6
15				GLU			103.929			1.00 20.00	
	ATOM	1194							-11.810		8
	ATOM	1195	OE2	GLU			103.344		-13.215	1.00 20.00	8
	MOTA	1196	С	GLU	В	215	101.275	22.307	-8.274	1.00 20.00	6
	MOTA	1197	0	GLU	В	215	101.801	21.205	-8.428	1.00 20.00	8
50	ATOM	1198	N	ASP			101.335	22.976	-7.123	1.00 20.00	7
50											
	MOTA	1199	CA	ASP			102.036	22.430	-5.958	1.00 20.00	6
	ATOM	1200	СВ	ASP	В	216	102.727	23.549	-5.179	1.00 20.00	6
	ATOM	1201	CG	ASP	В	216	103.952	24.086	-5.896	1.00 20.00	6
	ATOM	1202	OD1	ASP			104.766	23.267	-6.376	1.00 20.00	8
55	ATOM	1203		ASP			104.110	25.323	-5.973	1.00 20.00	8
55											
	ATOM	1204	С	ASP			101.121	21.651	-5.013	1.00 20.00	6
	ATOM	1205	0	ASP	В	216	101.532	21.241	-3.925	1.00 20.00	8
	ATOM	1206	N	MET	В	217	99.877	21.463	-5.434	1.00 20.00	7
	ATOM	1207	CA	MET			98.890	20.730	-4.657	1.00 20.00	6
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	MOTA	1208	СВ	MET			99.402	19.319	-4.358		20.00	6
	MOTA	1209	CG	MET			99.456	18.432	-5.601		20.00	6
	MOTA	1210	SD	MET	В	217	97.857	18.342	-6.445	1.00	20.00	16
	ATOM	1211	CE	MET	В	217	97.073	16.984	-5.543	1.00	20.00	6
5	ATOM	1212	С	MET	В	217	98.397	21.403	-3.373	1.00	20.00	6
	ATOM	1213	0	MET			97.972	20.730	-2.435		20.00	8
	ATOM	1214	N	HIS			98.469	22.730	-3.331		20.00	7
	ATOM	1215	CA	HIS			97.949	23.487	-2.197		20.00	6
1.0	ATOM	1216	СВ	HIS			98.831	24.700	-1.898		20.00	6
10	ATOM	1217	CG	HIS			100.100	24.357	-1.177		20.00	6
	MOTA	1218		HIS			101.390	24.362	-1.588		20.00	6
	ATOM	1219	ND1	HIS	В	218	100.117	23.935	0.136	1.00	20.00	7
	ATOM	1220	CE1	HIS	В	218	101.364	23.698	0.504	1.00	20.00	6
	ATOM	1221	NE2	HIS	В	218	102.156	23.947	-0.524	1.00	20.00	7
15	ATOM	1222	С	HIS			96.583	23.939	-2.703	1.00	20.00	6
	ATOM	1223	0	HIS			96.400	24.090	-3.910		20.00	8
	ATOM	1224	N	ILE			95.628	24.160	-1.808		20.00	7
		1225		ILE			94.301	24.562	-2.257		20.00	6
	ATOM		CA									
20	ATOM	1226	СВ	ILE			93.232	24.359	-1.159		20.00	6
20	ATOM	1227	CG2	ILE			93.266	22.918	-0.654		20.00	6
	ATOM	1228	CG1	ILE	В	219	93.460	25.353	-0.011	1.00	20.00	6
	MOTA	1229	CD1	ILE	В	219	92.351	25.342	1.036	1.00	20.00	6
	ATOM	1230	С	ILE	В	219	94.207	26.010	-2.714	1.00	20.00	6
	ATOM	1231	0	ILE	В	219	95.044	26.850	-2.375	1.00	20.00	8
25	ATOM	1232	N	GLN	В	220	93.168	26.274	-3.497	1.00	20.00	7
	ATOM	1233	CA	GLN			92.859	27.600	-3.999		20.00	6
	ATOM	1234	СВ	GLN			93.537	27.867	-5.350		20.00	6
	ATOM	1235	CG	GLN			95.011	28.246	-5.216		20.00	6
20	ATOM	1236	CD	GLN			95.599	28.799	-6.503		20.00	6
30	ATOM	1237		GLN			95.725	28.086	-7.502		20.00	8
	ATOM	1238		GLN			95.957	30.079	-6.486		20.00	7
	ATOM	1239	С	GLN			91.350	27.626	-4.140		20.00	6
	ATOM	1240	0	GLN	В	220	90.792	27.133	-5.124	1.00	20.00	8
	MOTA	1241	N	ILE	В	221	90.689	28.178	-3.129	1.00	20.00	7
35	ATOM	1242	CA	ILE	В	221	89.240	28.260	-3.122	1.00	20.00	6
	ATOM	1243	СВ	ILE	В	221	88.731	28.550	-1.700	1.00	20.00	6
	ATOM	1244	CG2	ILE			87.209	28.707	-1.708		20.00	6
	ATOM	1245	CG1	ILE			89.164	27.406	-0.773		20.00	6
	ATOM	1246	CD1	ILE			88.743	27.559	0.668		20.00	6
40		1247	CDI	ILE			88.760	29.339	-4.092		20.00	6
40	ATOM											
	ATOM	1248	0	ILE			89.411	30.374	-4.262		20.00	8
	ATOM	1249	N	THR			87.633				20.00	7
	MOTA	1250	CA	THR			87.084	30.039	-5.701		20.00	6
	ATOM	1251	СВ	THR	В	222	87.565	29.728	-7.125		20.00	6
45	ATOM	1252	OG1	THR	В	222	87.179	30.795	-8.000	1.00	20.00	8
	ATOM	1253	CG2	THR	В	222	86.962	28.410	-7.618	1.00	20.00	6
	ATOM	1254	С	THR	В	222	85.554	30.028	-5.683	1.00	20.00	6
	ATOM	1255	0	THR			84.950	29.417	-4.791		20.00	8
	ATOM	1256	N	ASP			84.949	30.712	-6.659		20.00	7
50	ATOM	1257	CA	ASP			83.492	30.806	-6.806		20.00	6
50	ATOM	1258	СВ	ASP			82.872	29.399	-6.767		20.00	6
	ATOM	1259	CG	ASP			81.414	29.384	-7.205		20.00	6
	ATOM	1260		ASP			80.990	30.335	-7.900		20.00	8
	MOTA	1261		ASP			80.701	28.414	-6.866		20.00	8
55	ATOM	1262	С	ASP			82.878	31.694	-5.725		20.00	6
	MOTA	1263	0	ASP	В	223	82.191	31.208	-4.820	1.00	20.00	8
	ATOM	1264	N	PHE	В	224	83.105	33.001	-5.848	1.00	20.00	7
	ATOM	1265	CA	PHE			82.632	33.970	-4.866		20.00	6
	ATOM	1266	СВ	PHE			83.800	34.869	-4.451		20.00	6
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	ATOM	1267	CG	PHE			84.826	34.165	-3.612	1.00 20.00	
	MOTA	1268	CD1	PHE	В	224	84.590	33.931	-2.261	1.00 20.00	
	ATOM	1269	CD2	PHE	В	224	86.001	33.687	-4.182	1.00 20.00) 6
	ATOM	1270	CE1	PHE	В	224	85.509	33.227	-1.486	1.00 20.00) 6
5	ATOM	1271	CE2	PHE			86.927	32.981	-3.418	1.00 20.00	
5		1272	CZ	PHE						1.00 20.00	
	ATOM						86.679	32.750	-2.068		
	ATOM	1273	С	PHE			81.443	34.839	-5.256	1.00 20.00	
	MOTA	1274	0	PHE	В	224	81.001	35.678	-4.468	1.00 20.00	8 (
	ATOM	1275	N	GLY	В	225	80.928	34.647	-6.463	1.00 20.00	7
10	ATOM	1276	CA	GLY	В	225	79.793	35.438	-6.894	1.00 20.00) 6
	ATOM	1277	С	GLY			78.612	35.265	-5.955	1.00 20.00	
		1278	0	GLY			77.824	36.192	-5.753	1.00 20.00	
	ATOM										
	ATOM	1279	N	THR			78.486	34.080	-5.367	1.00 20.00	
	ATOM	1280	CA	THR			77.379	33.819	-4.459	1.00 20.00) 6
15	MOTA	1281	CB	THR	В	226	76.779	32.425	-4.715	1.00 20.00) 6
	ATOM	1282	OG1	THR	В	226	77.826	31.450	-4.762	1.00 20.00	8 (
	ATOM	1283	CG2	THR	В	226	76.021	32.417	-6.041	1.00 20.00) 6
	ATOM	1284	C	THR			77.738	33.957	-2.981	1.00 20.00	
20	ATOM	1285	0	THR			77.001	33.500	-2.107	1.00 20.00	
20	ATOM	1286	N	ALA			78.867	34.598	-2.702	1.00 20.00	
	MOTA	1287	CA	ALA	В	227	79.282	34.800	-1.325	1.00 20.00) 6
	ATOM	1288	СВ	ALA	В	227	80.738	35.242	-1.268	1.00 20.00) 6
	ATOM	1289	С	ALA	В	227	78.384	35.875	-0.726	1.00 20.00) 6
	ATOM	1290	0	ALA			77.623	36.529	-1.440	1.00 20.00	
25	ATOM	1291		LYS			78.467	36.046	0.586	1.00 20.00	
23			N								
	ATOM	1292	CA	LYS			77.670	37.051	1.274	1.00 20.00	
	ATOM	1293	СВ	LYS			76.637	36.384	2.179	1.00 20.00	
	ATOM	1294	CG	LYS	В	228	75.705	37.357	2.890	1.00 20.00) 6
	MOTA	1295	CD	LYS	В	228	74.795	38.072	1.893	1.00 20.00) 6
30	MOTA	1296	CE	LYS	В	228	73.849	39.049	2.587	1.00 20.00) 6
	ATOM	1297	NΖ	LYS	В	228	73.000	39.781	1.605	1.00 20.00) 7
	ATOM	1298	C	LYS			78.616	37.896	2.110	1.00 20.00	
	ATOM	1299	0	LYS			79.355	37.366	2.940	1.00 20.00	
				VAL						1.00 20.00	
2.5	ATOM	1300	N				78.603	39.206	1.881		
35	ATOM	1301	CA	VAL			79.463	40.114	2.626	1.00 20.00	
	ATOM	1302	СВ	VAL	В	229	79.976	41.256	1.734	1.00 20.00) 6
	ATOM	1303	CG1	VAL	В	229	80.853	42.191	2.540	1.00 20.00) 6
	MOTA	1304	CG2	VAL	В	229	80.746	40.686	0.561	1.00 20.00) 6
	ATOM	1305	С	VAL	В	229	78.687	40.710	3.793	1.00 20.00) 6
40	ATOM	1306	0	VAL			77.798	41.537	3.599	1.00 20.00	
10	ATOM	1307	N	LEU			79.034	40.284	5.003	1.00 20.00	
	ATOM	1308	CA	LEU			78.370	40.752	6.213	1.00 20.00	
	ATOM	1309	СВ	LEU			78.740	39.856	7.395	1.00 20.00	
	ATOM	1310	CG	LEU			78.276	38.403	7.332	1.00 20.00	
45	MOTA	1311	CD1	LEU	В	230	78.853	37.634	8.508	1.00 20.00) 6
	ATOM	1312	CD2	LEU	В	230	76.760	38.350	7.339	1.00 20.00) 6
	ATOM	1313	С	LEU	В	230	78.705	42.193	6.565	1.00 20.00	
	ATOM	1314	0	LEU			79.768	42.701	6.214	1.00 20.00	
50	ATOM	1315	N	SER			77.781	42.839	7.270	1.00 20.00	
50	ATOM	1316	CA	SER			77.957	44.219	7.708	1.00 20.00	
	ATOM	1317	СВ	SER	В	231	77.082	45.161	6.875	1.00 20.00) 6
	MOTA	1318	OG	SER	В	231	75.714	44.795	6.948	1.00 20.00	8 (
	ATOM	1319	С	SER	В	231	77.623	44.373	9.196	1.00 20.00) 6
	ATOM	1320	0	SER			78.322	45.086	9.919	1.00 20.00	
55	ATOM	1321	N	PRO			76.553	43.705	9.674	1.00 20.00	
55											
	ATOM	1322	CD	PRO			75.571	42.876	8.948	1.00 20.00	
	ATOM	1323	CA	PRO			76.182	43.811	11.091	1.00 20.00	
	ATOM	1324	СВ	PRO			75.005	42.844	11.211	1.00 20.00	
	ATOM	1325	CG	PRO	В	232	74.367	42.933	9.862	1.00 20.00) 6

	7.001	1206	~	DD 0	_	0.2.0	77 220	42 420	10 001	1 00 00 00	_
	ATOM	1326	С	PRO			77.332	43.438	12.024	1.00 20.00	6
	MOTA	1327	0	PRO	В	232	78.199	42.640	11.666	1.00 20.00	8
	ATOM	1328	N	ALA	В	237	74.215	38.132	11.762	1.00 20.00	7
	ATOM	1329	CA	ALA	В	237	74.666	37.653	10.460	1.00 20.00	6
5	ATOM	1330	СВ	ALA			75.541	36.417	10.637	1.00 20.00	6
5		1331		ALA			73.479			1.00 20.00	
	ATOM		С					37.324	9.558		
	ATOM	1332	0	ALA			73.143	36.158	9.374	1.00 20.00	8
	MOTA	1333	N	ALA	В	238	72.841	38.347	8.996	1.00 20.00	7
	ATOM	1334	CA	ALA	В	238	71.693	38.130	8.117	1.00 20.00	6
10	ATOM	1335	СВ	ALA	В	238	70.973	39.450	7.853	1.00 20.00	6
	ATOM	1336	С	ALA			72.123	37.497	6.798	1.00 20.00	6
											8
	ATOM	1337	0	ALA			73.315	37.404	6.500	1.00 20.00	
	ATOM	1338	N	ALA			71.146	37.057	6.012	1.00 20.00	7
	MOTA	1339	CA	ALA			71.439	36.431	4.728	1.00 20.00	6
15	ATOM	1340	СВ	ALA	В	239	72.152	35.123	4.952	1.00 20.00	6
	ATOM	1341	С	ALA	В	239	70.173	36.194	3.918	1.00 20.00	6
	ATOM	1342	0	ALA			69.329	37.079	3.825	1.00 20.00	8
								34.996		1.00 20.00	7
	ATOM	1343	N	ASN			70.068		3.339		
	ATOM	1344	CA	ASN			68.939	34.559	2.514	1.00 20.00	
20	ATOM	1345	СВ	ASN	В	240	67.614	35.160	2.999	1.00 20.00	6
	ATOM	1346	CG	ASN	В	240	67.258	36.466	2.299	1.00 20.00	6
	ATOM	1347	OD1	ASN	В	240	67.119	36.519	1.068	1.00 20.00	8
	ATOM	1348		ASN			67.091	37.536	3.089	1.00 20.00	
	ATOM	1349	C	ASN			69.153	34.937	1.053	1.00 20.00	
25											
25	ATOM	1350	0	ASN			70.007	35.767	0.749	1.00 20.00	8
	ATOM	1351	N	ALA			68.365	34.329	0.163	1.00 20.00	
	MOTA	1352	CA	ALA	В	241	68.401	34.570	-1.290	1.00 20.00	6
	ATOM	1353	С	ALA	В	241	68.990	33.416	-2.103	1.00 20.00	6
	ATOM	1354	0	ALA	В	241	68.353	32.919	-3.030	1.00 20.00	8
30	ATOM	1355	СВ	ALA			69.168	35.859	-1.629	1.00 20.00	6
30		1356						33.000			7
	ATOM		N	PHE			70.205		-1.762	1.00 20.00	
	ATOM	1357	CA	PHE			70.875	31.918	-2.481	1.00 20.00	
	ATOM	1358	CB	PHE	В	242	72.259	32.379	-2.952	1.00 20.00	6
	MOTA	1359	CG	PHE	В	242	73.102	31.273	-3.521	1.00 20.00	6
35	ATOM	1360	CD1	PHE	В	242	72.843	30.767	-4.790	1.00 20.00	6
	ATOM	1361	CD2	PHE	В	242	74.136	30.713	-2.773	1.00 20.00	
	ATOM	1362		PHE			73.599	29.718	-5.310	1.00 20.00	
	ATOM	1363	CE2	PHE			74.896	29.666	-3.281	1.00 20.00	6
	ATOM	1364	CZ	PHE			74.627	29.166	-4.553	1.00 20.00	6
40	MOTA	1365	С	PHE	В	242	71.038	30.652	-1.646	1.00 20.00	6
	ATOM	1366	0	PHE	В	242	71.213	30.716	-0.431	1.00 20.00	8
	MOTA	1367	N	VAL	В	243	70.988	29.505	-2.318	1.00 20.00	7
	ATOM	1368	CA	VAL			71.157	28.204	-1.675	1.00 20.00	6
	ATOM	1369	СВ	VAL			69.828	27.420	-1.617	1.00 20.00	6
15											
45	ATOM	1370		VAL			70.066	26.023	-1.050	1.00 20.00	6
	ATOM	1371	CG2	VAL			68.825	28.177	-0.766	1.00 20.00	6
	MOTA	1372	С	VAL	В	243	72.164	27.394	-2.486	1.00 20.00	6
	ATOM	1373	0	VAL	В	243	71.894	27.014	-3.628	1.00 20.00	8
	ATOM	1374	N	GLY	В	244	73.323	27.137	-1.890	1.00 20.00	7
50	ATOM	1375	CA	GLY			74.364	26.385	-2.569	1.00 20.00	6
50	ATOM	1376		GLY						1.00 20.00	
			C				74.019	24.944	-2.911		6
	ATOM	1377	0	GLY			72.867	24.524	-2.810	1.00 20.00	8
	MOTA	1378	N	THR			75.032	24.184	-3.315	1.00 20.00	7
	ATOM	1379	CA	THR	В	245	74.858	22.787	-3.691	1.00 20.00	6
55	ATOM	1380	СВ	THR			76.214	22.161	-4.046	1.00 20.00	6
	ATOM	1381		THR			76.794	22.911	-5.120	1.00 20.00	8
		1382						20.710			6
	ATOM			THR			76.049		-4.485	1.00 20.00	
	ATOM	1383	С	THR			74.174	22.003	-2.579	1.00 20.00	6
	ATOM	1384	0	THR	В	245	74.643	21.969	-1.441	1.00 20.00	8

	MOTA	1385	Ν	ALA	В	246	73.061	21.372	-2.937	1.00 20.00	7
	ATOM	1386	CA	ALA	В	246	72.229	20.615	-2.008	1.00 20.00	6
	ATOM	1387	СВ	ALA	В	246	71.266	19.723	-2.793	1.00 20.00	6
	ATOM	1388	C	ALA			72.936	19.789	-0.941	1.00 20.00	6
5	ATOM	1389	0	ALA			72.611	19.894	0.239	1.00 20.00	8
)											
	ATOM	1390	N	GLN			73.902	18.973	-1.339	1.00 20.00	7
	ATOM	1391	CA	GLN	В	247	74.580	18.121	-0.371	1.00 20.00	6
	ATOM	1392	CB	GLN	В	247	75.535	17.168	-1.096	1.00 20.00	6
	ATOM	1393	CG	GLN	В	247	75.110	16.823	-2.520	1.00 20.00	6
10	ATOM	1394	CD	GLN	В	247	75.139	15.336	-2.811	1.00 20.00	6
10	ATOM	1395		GLN			75.963	14.602	-2.270	1.00 20.00	8
	ATOM	1396	NE2	GLN			74.246	14.887	-3.686	1.00 20.00	7
	ATOM	1397	С	GLN			75.343	18.873	0.720	1.00 20.00	6
	MOTA	1398	0	GLN	В	247	75.631	18.306	1.773	1.00 20.00	8
15	MOTA	1399	N	TYR	В	248	75.648	20.147	0.484	1.00 20.00	7
	ATOM	1400	CA	TYR	В	248	76.405	20.941	1.454	1.00 20.00	6
	ATOM	1401	СВ	TYR			77.642	21.531	0.767	1.00 20.00	6
		1402	CG	TYR			78.447	20.471	0.052	1.00 20.00	6
	ATOM										
	ATOM	1403		TYR			79.329	19.648	0.750	1.00 20.00	6
20	ATOM	1404	CE1	TYR	В	248	79.979	18.589	0.115	1.00 20.00	6
	MOTA	1405	CD2	TYR	В	248	78.243	20.220	-1.306	1.00 20.00	6
	MOTA	1406	CE2	TYR	В	248	78.884	19.167	-1.951	1.00 20.00	6
	ATOM	1407	CZ	TYR	В	248	79.748	18.352	-1.232	1.00 20.00	6
	ATOM	1408	ОН	TYR	В	248	80.348	17.280	-1.852	1.00 20.00	8
25	ATOM	1409	C	TYR			75.596	22.055	2.118	1.00 20.00	6
23	ATOM	1410	0	TYR			76.132	22.824	2.917	1.00 20.00	8
	ATOM	1411	N	VAL			74.309	22.135	1.798	1.00 20.00	7
	ATOM	1412	CA	VAL			73.452	23.162	2.376	1.00 20.00	6
	ATOM	1413	СВ	VAL			72.071	23.174	1.695	1.00 20.00	6
30	MOTA	1414	CG1	VAL	В	249	71.117	24.100	2.442	1.00 20.00	6
	ATOM	1415	CG2	VAL	В	249	72.225	23.632	0.264	1.00 20.00	6
	MOTA	1416	С	VAL	В	249	73.262	22.964	3.875	1.00 20.00	6
	ATOM	1417	0	VAL	В	249	73.027	21.847	4.341	1.00 20.00	8
	ATOM	1418	N	SER			73.373	24.055	4.628	1.00 20.00	7
35	ATOM	1419	CA	SER			73.206	24.008	6.076	1.00 20.00	6
55	ATOM	1420	CB	SER			73.921	25.198	6.738	1.00 20.00	6
	ATOM	1421	OG	SER			73.428	26.440	6.257	1.00 20.00	8
	ATOM	1422	С	SER			71.717	24.049	6.405	1.00 20.00	6
	MOTA	1423	0	SER	В	250	70.920	24.577	5.636	1.00 20.00	8
40	ATOM	1424	N	PRO	В	251	71.322	23.479	7.550	1.00 20.00	7
	MOTA	1425	CD	PRO	В	251	72.130	22.770	8.558	1.00 20.00	6
	ATOM	1426	CA	PRO	В	251	69.905	23.484	7.925	1.00 20.00	6
	ATOM	1427	СВ	PRO			69.892	22.714	9.252	1.00 20.00	6
	ATOM	1428	CG	PRO			71.290		9.801	1.00 20.00	6
45	ATOM	1429	C	PRO			69.265	24.870	8.032	1.00 20.00	6
43											
	ATOM	1430	0	PRO			68.093	25.036	7.688	1.00 20.00	8
	ATOM	1431	N	GLU			70.017	25.867	8.492	1.00 20.00	7
	ATOM	1432	CA	GLU	В	252	69.462	27.216	8.625	1.00 20.00	6
	MOTA	1433	CB	GLU	В	252	70.503	28.193	9.196	1.00 20.00	6
50	ATOM	1434	CG	GLU	В	252	71.838	28.180	8.477	1.00 20.00	6
	ATOM	1435	CD	GLU	В	252	72.844	27.257	9.139	1.00 20.00	6
	ATOM	1436	OE 1	GLU			72.429	26.207	9.675	1.00 20.00	8
	ATOM	1437		GLU			74.053	27.581	9.118	1.00 20.00	8
<i>5 5</i>	ATOM	1438	C	GLU			68.928	27.744	7.292	1.00 20.00	6
55	ATOM	1439	0	GLU			67.927	28.459	7.261	1.00 20.00	8
	ATOM	1440	N	LEU			69.584	27.395	6.189	1.00 20.00	7
	ATOM	1441	CA	LEU			69.117	27.850	4.883	1.00 20.00	6
	ATOM	1442	СВ	LEU	В	253	70.140	27.527	3.794	1.00 20.00	6
	ATOM	1443	CG	LEU	В	253	71.127	28.635	3.421	1.00 20.00	6

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	ATOM	1444	CD1	LEU	В	253	72.121	28.851	4.547	1.00	20.00	6
	ATOM	1445	CD2	LEU	В	253	71.858	28.250	2.140	1.00	20.00	6
	ATOM	1446	С	LEU	В	253	67.774	27.227	4.496	1.00	20.00	6
	ATOM	1447	0	LEU	В	253	66.997	27.826	3.751	1.00	20.00	8
5	ATOM	1448	N	LEU			67.506	26.029	5.002		20.00	7
5												
	MOTA	1449	CA	LEU			66.271	25.316	4.689		20.00	6
	ATOM	1450	СВ	LEU			66.539	23.809	4.689		20.00	6
	ATOM	1451	CG	LEU	В	254	67.647	23.322	3.746	1.00	20.00	6
	ATOM	1452	CD1	LEU	В	254	67.983	21.873	4.057	1.00	20.00	6
10	ATOM	1453		LEU			67.204	23.475	2.302	1.00	20.00	6
	ATOM	1454	C	LEU			65.135	25.626	5.662		20.00	6
				LEU								8
	ATOM	1455	0				63.959	25.524	5.312		20.00	
	MOTA	1456	N	THR			65.483	26.010	6.883		20.00	7
	ATOM	1457	CA	THR	В	255	64.472	26.308	7.884	1.00	20.00	6
15	ATOM	1458	СВ	THR	В	255	64.876	25.747	9.252	1.00	20.00	6
	ATOM	1459	OG1	THR	В	255	66.154	26.277	9.619	1.00	20.00	8
	ATOM	1460	CG2	THR	В	255	64.958	24.230	9.202	1.00	20.00	6
	ATOM	1461	C	THR			64.205	27.795	8.035		20.00	6
20	ATOM	1462	0	THR			63.072	28.241	7.897		20.00	8
20	MOTA	1463	Ν	GLU			65.250	28.560	8.314		20.00	7
	ATOM	1464	CA	GLU	В	256	65.115	30.001	8.507	1.00	20.00	6
	ATOM	1465	СВ	GLU	В	256	66.015	30.444	9.659	1.00	20.00	6
	ATOM	1466	CG	GLU	В	256	65.634	29.818	10.987	1.00	20.00	6
	ATOM	1467	CD	GLU	В	256	66.736	29.922	12.018	1.00	20.00	6
25	ATOM	1468	OE1	GLU			67.249	31.041	12.232		20.00	8
23	ATOM	1469	OE2	GLU			67.086	28.884	12.619		20.00	8
		1470		GLU			65.439	30.815	7.262		20.00	6
	ATOM		C									
	ATOM	1471	0	GLU			65.268	32.034	7.252		20.00	8
	MOTA	1472	N	LYS			65.906	30.141	6.215		20.00	7
30	ATOM	1473	CA	LYS	В	257	66.260	30.814	4.970	1.00	20.00	6
	ATOM	1474	CB	LYS	В	257	65.015	31.458	4.352	1.00	20.00	6
	ATOM	1475	CG	LYS	В	257	65.184	31.918	2.915	1.00	20.00	6
	ATOM	1476	CD	LYS	В	257	63.885	32.497	2.378	1.00	20.00	6
	ATOM	1477	CE	LYS			63.994	32.841	0.902		20.00	6
35	ATOM	1478	NZ	LYS			65.060	33.847	0.640		20.00	7
33			C	LYS							20.00	
	ATOM	1479					67.309	31.885	5.263			6
	MOTA	1480	0	LYS			67.270	32.977	4.702		20.00	8
	ATOM	1481	N	SER			68.243	31.563	6.152		20.00	7
	ATOM	1482	CA	SER			69.300	32.494	6.527	1.00	20.00	6
40	ATOM	1483	CB	SER	В	258	69.043	33.028	7.937	1.00	20.00	6
	ATOM	1484	OG	SER	В	258	68.893	31.962	8.859	1.00	20.00	8
	ATOM	1485	С	SER	В	258	70.675	31.829	6.467	1.00	20.00	6
	ATOM	1486	0	SER			70.786	30.602	6.542		20.00	8
	ATOM	1487	N	ALA			71.718	32.641	6.329		20.00	7
45		1488									20.00	
43	ATOM		CA	ALA			73.081	32.130	6.252			6
	MOTA	1489	СВ	ALA			73.549	32.121	4.809		20.00	6
	MOTA	1490	С	ALA			74.031	32.966	7.102		20.00	6
	ATOM	1491	0	ALA			73.882	34.185	7.211	1.00	20.00	8
	ATOM	1492	N	CYS	В	260	75.008	32.298	7.704	1.00	20.00	7
50	MOTA	1493	CA	CYS			75.993	32.960	8.550	1.00	20.00	6
	MOTA	1494	СВ	CYS			75.574	32.865	10.017		20.00	6
	ATOM	1495	SG	CYS			75.303	31.165	10.594		20.00	16
	MOTA	1496	С	CYS			77.328	32.265	8.349		20.00	6
	MOTA	1497	0	CYS			77.410	31.280	7.620		20.00	8
55	ATOM	1498	N	LYS	В	261	78.371	32.775	8.993	1.00	20.00	7
	ATOM	1499	CA	LYS	В	261	79.691	32.174	8.869	1.00	20.00	6
	MOTA	1500	СВ	LYS			80.676	32.851	9.821	1.00	20.00	6
	ATOM	1501	CG	LYS			80.985	34.296	9.472		20.00	6
	ATOM	1502	CD	LYS			81.961	34.878	10.475		20.00	6
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	ATOM	1503	CE	LYS	В	261	82.157	36.365	10.259	1.00 20.00	6
	ATOM	1504	NZ	LYS	В	261	83.085	36.922	11.278	1.00 20.00	7
	ATOM	1505	С	LYS	В	261	79.632	30.687	9.187	1.00 20.00	6
	ATOM	1506	0	LYS	В	261	80.258	29.877	8.512	1.00 20.00	8
5	ATOM	1507	N	SER			78.860	30.346	10.214	1.00 20.00	7
5											
	MOTA	1508	CA	SER			78.716	28.966	10.659	1.00 20.00	6
	MOTA	1509	СВ	SER			77.806	28.913	11.895	1.00 20.00	6
	ATOM	1510	OG	SER	В	262	77.884	27.657	12.546	1.00 20.00	8
	ATOM	1511	С	SER	В	262	78.161	28.070	9.549	1.00 20.00	6
10	ATOM	1512	0	SER			78.350	26.856	9.575	1.00 20.00	8
	ATOM	1513	N	SER			77.466	28.660	8.581	1.00 20.00	7
	MOTA	1514	CA	SER			76.938	27.870	7.472	1.00 20.00	6
	MOTA	1515	СВ	SER			76.132	28.750	6.507	1.00 20.00	6
	ATOM	1516	OG	SER	В	263	75.011	29.329	7.156	1.00 20.00	8
15	ATOM	1517	С	SER	В	263	78.123	27.244	6.737	1.00 20.00	6
	ATOM	1518	0	SER	В	263	78.038	26.108	6.273	1.00 20.00	8
	ATOM	1519	N	ASP			79.234	27.977	6.642	1.00 20.00	7
	ATOM	1520	CA	ASP			80.419	27.448	5.961	1.00 20.00	6
	MOTA	1521	СВ	ASP	В	264	81.478	28.538	5.745	1.00 20.00	6
20	ATOM	1522	CG	ASP	В	264	81.091	29.539	4.673	1.00 20.00	6
	ATOM	1523	OD1	ASP	В	264	80.286	29.187	3.786	1.00 20.00	8
	ATOM	1524	OD2	ASP	В	264	81.617	30.676	4.704	1.00 20.00	8
	MOTA	1525	С	ASP			81.043	26.312	6.771	1.00 20.00	6
	ATOM	1526		ASP			81.586	25.365	6.201	1.00 20.00	8
25			0								
25	MOTA	1527	N	LEU			80.971	26.415	8.099	1.00 20.00	7
	ATOM	1528	CA	LEU	В	265	81.532	25.390	8.974	1.00 20.00	6
	ATOM	1529	СВ	LEU	В	265	81.491	25.848	10.438	1.00 20.00	6
	ATOM	1530	CG	LEU	В	265	82.419	27.035	10.746	1.00 20.00	6
	ATOM	1531	CD1	LEU	В	265	82.204	27.532	12.177	1.00 20.00	6
30	ATOM	1532		LEU			83.864	26.608	10.541	1.00 20.00	6
30											
	ATOM	1533	С	LEU			80.750	24.094	8.800	1.00 20.00	6
	ATOM	1534	0	LEU			81.306	23.004	8.910	1.00 20.00	8
	ATOM	1535	N	TRP	В	266	79.454	24.208	8.530	1.00 20.00	7
	MOTA	1536	CA	TRP	В	266	78.646	23.017	8.309	1.00 20.00	6
35	ATOM	1537	СВ	TRP	В	266	77.167	23.384	8.148	1.00 20.00	6
	ATOM	1538	CG	TRP			76.310	22.245	7.646	1.00 20.00	6
	ATOM	1539	CD2	TRP			75.455	21.399	8.426	1.00 20.00	6
	ATOM	1540	CE2	TRP			74.881	20.455	7.542	1.00 20.00	6
	MOTA	1541	CE3	TRP			75.117	21.345	9.785	1.00 20.00	6
40	MOTA	1542	CD1	TRP	В	266	76.220	21.792	6.356	1.00 20.00	6
	ATOM	1543	NE1	TRP	В	266	75.365	20.719	6.288	1.00 20.00	7
	ATOM	1544	CZ2	TRP	В	266	73.988	19.466	7.975	1.00 20.00	6
	ATOM	1545		TRP			74.227	20.359	10.216	1.00 20.00	6
	ATOM	1546		TRP			73.674	19.434	9.310	1.00 20.00	6
15											
45	ATOM	1547	С	TRP			79.169	22.356	7.038	1.00 20.00	6
	MOTA	1548	0	TRP			79.356	21.142	6.988	1.00 20.00	8
	ATOM	1549	Ν	ALA	В	267	79.411	23.164	6.011	1.00 20.00	7
	ATOM	1550	CA	ALA	В	267	79.930	22.646	4.751	1.00 20.00	6
	MOTA	1551	СВ	ALA	В	267	80.089	23.772	3.746	1.00 20.00	6
50	ATOM	1552	С	ALA			81.277	21.976	5.016	1.00 20.00	6
20	ATOM	1553	0	ALA			81.570	20.914	4.471	1.00 20.00	8
	ATOM	1554	N	LEU			82.091	22.596	5.864	1.00 20.00	7
	ATOM	1555	CA	LEU	В	268	83.393	22.030	6.209	1.00 20.00	6
	ATOM	1556	СВ	LEU	В	268	84.092	22.898	7.264	1.00 20.00	6
55	ATOM	1557	CG	LEU	В	268	85.379	22.332	7.879	1.00 20.00	6
	MOTA	1558		LEU			86.442	22.192	6.803	1.00 20.00	6
	ATOM	1559		LEU			85.872	23.263	9.006	1.00 20.00	6
	ATOM	1560	C	LEU			83.193	20.617	6.753	1.00 20.00	6
	ATOM	1561	0	LEU	В	268	83.903	19.684	6.372	1.00 20.00	8

	MOTA	1562	N	GLY	В	269	82.220	20.463	7.645	1.00	20.00	7
	ATOM	1563	CA	GLY	В	269	81.947	19.156	8.217	1.00	20.00	6
	ATOM	1564	С	GLY	В	269	81.597	18.125	7.156	1.00	20.00	6
	ATOM	1565	0	GLY			82.025	16.971	7.239		20.00	8
5												
3	ATOM	1566	N	CYS			80.819	18.530	6.155		20.00	7
	ATOM	1567	CA	CYS			80.445	17.613	5.083		20.00	6
	ATOM	1568	СВ	CYS	В	270	79.413	18.255	4.148	1.00	20.00	6
	ATOM	1569	SG	CYS	В	270	77.824	18.654	4.905	1.00	20.00	16
	ATOM	1570	С	CYS	В	270	81.682	17.241	4.265	1.00	20.00	6
10	ATOM	1571	0	CYS			81.852	16.090	3.866	1.00	20.00	8
	ATOM	1572	N	ILE			82.541	18.226	4.012		20.00	7
	MOTA	1573	CA	ILE			83.751	18.000	3.229		20.00	6
	ATOM	1574	СВ	ILE			84.436	19.339	2.903		20.00	6
	ATOM	1575	CG2	ILE	В	271	85.784	19.098	2.227	1.00	20.00	6
15	ATOM	1576	CG1	ILE	В	271	83.508	20.171	2.007	1.00	20.00	6
	ATOM	1577	CD1	ILE	В	271	83.962	21.607	1.815	1.00	20.00	6
	ATOM	1578	С	ILE			84.729	17.063	3.934		20.00	6
	ATOM	1579	0	ILE			85.300	16.174	3.304		20.00	8
												7
20	ATOM	1580	N	ILE			84.927	17.258	5.236		20.00	
20	ATOM	1581	CA	ILE			85.820	16.382	5.987		20.00	6
	ATOM	1582	СВ	ILE			85.902	16.790	7.471		20.00	6
	ATOM	1583	CG2	ILE	В	272	86.623	15.703	8.277	1.00	20.00	6
	MOTA	1584	CG1	ILE	В	272	86.646	18.120	7.606	1.00	20.00	6
	ATOM	1585	CD1	ILE	В	272	86.553	18.723	9.011	1.00	20.00	6
25	ATOM	1586	С	ILE	В	272	85.274	14.957	5.901	1.00	20.00	6
	ATOM	1587	0	ILE	В	272	86.021	14.003	5.679	1.00	20.00	8
	ATOM	1588	N	TYR			83.964	14.822	6.072		20.00	7
	ATOM	1589	CA	TYR			83.324	13.518	6.006		20.00	6
		1590	CB	TYR			81.825	13.651	6.287		20.00	6
20	ATOM											
30	ATOM	1591	CG	TYR			81.064	12.340	6.250		20.00	6
	ATOM	1592		TYR			80.806	11.690	5.041		20.00	6
	ATOM	1593		TYR			80.107	10.486	5.005		20.00	6
	ATOM	1594	CD2	TYR			80.601	11.750	7.427	1.00	20.00	6
	ATOM	1595	CE2	TYR	В	273	79.904	10.548	7.405	1.00	20.00	6
35	MOTA	1596	CZ	TYR	В	273	79.659	9.922	6.192	1.00	20.00	6
	ATOM	1597	OH	TYR	В	273	78.971	8.736	6.174	1.00	20.00	8
	ATOM	1598	С	TYR	В	273	83.550	12.897	4.632	1.00	20.00	6
	ATOM	1599	0	TYR			83.865	11.713	4.526		20.00	8
	ATOM	1600	N	GLN			83.402	13.705	3.586		20.00	7
40		1601		GLN			83.579	13.703	2.220		20.00	6
40	ATOM		CA									
	ATOM	1602	СВ	GLN			83.176	14.322	1.222		20.00	6
	MOTA	1603		GLN				13.857				
	ATOM	1604	CD	GLN			82.558	14.898	-1.169		20.00	6
	ATOM	1605	OE1	GLN	В	274	82.108	15.961		1.00	20.00	8
45	ATOM	1606	NE2	GLN	В	274	82.548	14.591	-2.462	1.00	20.00	7
	ATOM	1607	С	GLN	В	274	85.013	12.788	1.953	1.00	20.00	6
	ATOM	1608	0	GLN			85.239	11.818	1.233	1.00	20.00	8
	ATOM	1609	N	LEU	В	275	85.981	13.498	2.528	1.00	20.00	7
	ATOM	1610	CA	LEU			87.389	13.143	2.333		20.00	6
50	ATOM	1611	СВ	LEU			88.311	14.194	2.971		20.00	6
50		1612		LEU								
	ATOM		CG				88.418	15.561	2.284		20.00	6
	MOTA	1613		LEU			89.325	16.481	3.088		20.00	6
	ATOM	1614		LEU			88.969	15.379	0.879		20.00	6
	MOTA	1615	С	LEU			87.697	11.779	2.940		20.00	6
55	MOTA	1616	0	LEU	В	275	88.430	10.981	2.354	1.00	20.00	8
	MOTA	1617	N	VAL	В	276	87.125	11.519	4.112	1.00	20.00	7
	ATOM	1618	CA	VAL	В	276	87.353	10.269	4.827	1.00	20.00	6
	ATOM	1619	СВ	VAL			87.096	10.451	6.342		20.00	6
	ATOM	1620		VAL			87.376	9.148	7.082		20.00	6
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	ATOM	1621		VAL			87.973	11.580	6.891	1.00 20.00	6
	ATOM	1622	С	VAL			86.504	9.089	4.336	1.00 20.00	6
	ATOM	1623	0	VAL	В	276	87.005	7.973	4.195	1.00 20.00	8
	ATOM	1624	N	ALA	В	277	85.222	9.337	4.090	1.00 20.00	7
5	ATOM	1625	CA	ALA			84.310	8.291	3.643	1.00 20.00	6
5		1626		ALA			82.898			1.00 20.00	
	ATOM		СВ					8.597	4.124		6
	ATOM	1627	С	ALA			84.315	8.115	2.130	1.00 20.00	6
	MOTA	1628	0	ALA	В	277	84.036	7.029	1.627	1.00 20.00	8
	ATOM	1629	N	GLY	В	278	84.632	9.180	1.405	1.00 20.00	7
10	ATOM	1630	CA	GLY			84.653	9.099	-0.041	1.00 20.00	6
10	ATOM	1631	C	GLY			83.365	9.627	-0.644	1.00 20.00	6
	MOTA	1632	0	GLY			83.272	9.817	-1.860	1.00 20.00	8
	MOTA	1633	N	LEU	В	279	82.375	9.867	0.211	1.00 20.00	7
	ATOM	1634	CA	LEU	В	279	81.075	10.382	-0.219	1.00 20.00	6
15	ATOM	1635	СВ	LEU	В	279	80.070	9.232	-0.375	1.00 20.00	6
	ATOM	1636	CG	LEU			80.342	8.114	-1.385	1.00 20.00	6
		1637		LEU			79.311	7.009	-1.191	1.00 20.00	6
	ATOM										
	ATOM	1638	CD2	LEU			80.291	8.660	-2.804	1.00 20.00	6
	ATOM	1639	С	LEU	В	279	80.522	11.369	0.812	1.00 20.00	6
20	ATOM	1640	0	LEU	В	279	80.750	11.218	2.007	1.00 20.00	8
	ATOM	1641	N	PRO	В	280	79.787	12.395	0.361	1.00 20.00	7
	ATOM	1642	CD	PRO			79.403	12.730	-1.020	1.00 20.00	6
	ATOM	1643	CA	PRO			79.230	13.361	1.314	1.00 20.00	6
	ATOM	1644	СВ	PRO			78.569	14.397	0.407	1.00 20.00	6
25	ATOM	1645	CG	PRO	В	280	78.191	13.598	-0.802	1.00 20.00	6
	MOTA	1646	С	PRO	В	280	78.242	12.662	2.262	1.00 20.00	6
	ATOM	1647	0	PRO	В	280	77.666	11.633	1.913	1.00 20.00	8
	ATOM	1648	N	PRO			78.035	13.220	3.470	1.00 20.00	7
											6
20	ATOM	1649	CD	PRO			78.571	14.535	3.859	1.00 20.00	
30	ATOM	1650	CA	PRO			77.145	12.701	4.520	1.00 20.00	6
	MOTA	1651	СВ	PRO	В	281	77.262	13.746	5.634	1.00 20.00	6
	ATOM	1652	CG	PRO	В	281	78.546	14.450	5.344	1.00 20.00	6
	ATOM	1653	С	PRO	В	281	75.679	12.485	4.142	1.00 20.00	6
	ATOM	1654	0	PRO			75.094	11.441	4.442	1.00 20.00	8
25											
35	ATOM	1655	N	PHE			75.088	13.487	3.504	1.00 20.00	7
	ATOM	1656	CA	PHE			73.686	13.427	3.123	1.00 20.00	6
	ATOM	1657	СВ	PHE	В	282	73.006	14.734	3.531	1.00 20.00	6
	MOTA	1658	CG	PHE	В	282	73.300	15.146	4.947	1.00 20.00	6
	ATOM	1659	CD1	PHE	В	282	72.624	14.560	6.013	1.00 20.00	6
40	ATOM	1660	CD2	PHE	В	282	74.295	16.085	5.218	1.00 20.00	6
10	ATOM	1661		PHE			72.934	14.902	7.331	1.00 20.00	6
	ATOM	1662		PHE			74.613			1.00 20.00	6
	MOTA	1663	CZ	PHE			73.930	15.840	7.591	1.00 20.00	6
	MOTA	1664	С	PHE	В	282	73.527	13.191	1.628	1.00 20.00	6
45	ATOM	1665	0	PHE	В	282	73.797	14.079	0.819	1.00 20.00	8
	ATOM	1666	N	ARG			73.080	11.994	1.267	1.00 20.00	7
	ATOM	1667	CA	ARG			72.888	11.635	-0.134	1.00 20.00	6
							73.931				
	ATOM	1668	СВ	ARG				10.598	-0.559	1.00 20.00	6
	ATOM	1669	CG	ARG			75.358	10.928	-0.151	1.00 20.00	6
50	ATOM	1670	CD	ARG	В	283	76.326	9.883	-0.687	1.00 20.00	6
	ATOM	1671	NE	ARG	В	283	76.054	8.555	-0.142	1.00 20.00	7
	ATOM	1672	CZ	ARG			76.404	8.159	1.077	1.00 20.00	6
	ATOM	1673		ARG			77.047	8.986	1.893	1.00 20.00	7
	ATOM	1674		ARG			76.108	6.933	1.484	1.00 20.00	7
55	ATOM	1675	С	ARG			71.493	11.046	-0.331	1.00 20.00	6
	ATOM	1676	0	ARG	В	283	70.957	10.391	0.563	1.00 20.00	8
	ATOM	1677	N	ALA	В	284	70.911	11.276	-1.502	1.00 20.00	7
	ATOM	1678	CA	ALA			69.579	10.755	-1.796	1.00 20.00	6
	ATOM	1679	CB	ALA			68.532	11.484	-0.961	1.00 20.00	6
	AT OM	T0/2	CD	ΑπΑ	נו	4 U H	00.334	TT.404	-0.96T	1.00 20.00	О

	ATOM	1600	C	71 71	D	201	60 270	10 021	_ 2 272	1.00 20.00	6
		1680	C	ALA			69.278	10.921	-3.273		6
	ATOM	1681	0	ALA			70.007	11.611	-3.984	1.00 20.00	8
	ATOM	1682	N	GLY			68.191	10.299	-3.722	1.00 20.00	7
	ATOM	1683	CA	GLY			67.807	10.360	-5.122	1.00 20.00	6
5	MOTA	1684	С	$\operatorname{GL} Y$	В	285	67.561	11.737	-5.707	1.00 20.00	6
	ATOM	1685	0	GLY	В	285	67.775	11.955	-6.899	1.00 20.00	8
	MOTA	1686	N	ASN	В	286	67.089	12.673	-4.892	1.00 20.00	7
	ATOM	1687	CA	ASN	В	286	66.835	14.018	-5.386	1.00 20.00	6
	ATOM	1688	СВ	ASN	В	286	65.403	14.137	-5.930	1.00 20.00	6
10	ATOM	1689	CG	ASN			64.342	13.825	-4.885	1.00 20.00	6
10	ATOM	1690		ASN			64.292	14.450	-3.826	1.00 20.00	8
								12.861			7
	ATOM	1691		ASN			63.477		-5.190	1.00 20.00	
	ATOM	1692	С	ASN			67.076	15.042	-4.291	1.00 20.00	6
	ATOM	1693	0	ASN			67.368	14.682	-3.152	1.00 20.00	8
15	ATOM	1694	N	GLU			66.955	16.317	-4.636	1.00 20.00	7
	MOTA	1695	CA	GLU	В	287	67.185	17.377	-3.669	1.00 20.00	6
	ATOM	1696	СВ	GLU	В	287	67.181	18.738	-4.365	1.00 20.00	6
	MOTA	1697	CG	GLU	В	287	68.537	19.095	-4.944	1.00 20.00	6
	ATOM	1698	CD	GLU	В	287	68.524	20.385	-5.735	1.00 20.00	6
20	ATOM	1699	OE 1	GLU	В	287	67.911	21.371	-5.267	1.00 20.00	8
	ATOM	1700	OE2	GLU			69.144	20.410	-6.823	1.00 20.00	8
	ATOM	1701	C	GLU			66.225	17.394	-2.492	1.00 20.00	6
		1702	0	GLU			66.658	17.554	-1.354	1.00 20.00	8
	ATOM										
25	ATOM	1703	N	TYR			64.932	17.233	-2.753	1.00 20.00	7
25	ATOM	1704	CA	TYR			63.955	17.239	-1.670	1.00 20.00	6
	ATOM	1705	СВ	TYR			62.553	16.899	-2.184	1.00 20.00	6
	ATOM	1706	CG	TYR			61.530	16.780	-1.070	1.00 20.00	6
	ATOM	1707	CD1	TYR	В	288	60.984	17.917	-0.470	1.00 20.00	6
	ATOM	1708	CE1	TYR	В	288	60.090	17.814	0.600	1.00 20.00	6
30	ATOM	1709	CD2	TYR	В	288	61.154	15.529	-0.573	1.00 20.00	6
	MOTA	1710	CE2	TYR	В	288	60.265	15.414	0.498	1.00 20.00	6
	ATOM	1711	CZ	TYR	В	288	59.740	16.561	1.078	1.00 20.00	6
	ATOM	1712	ОН	TYR	В	288	58.884	16.454	2.149	1.00 20.00	8
	ATOM	1713	С	TYR			64.337	16.238	-0.587	1.00 20.00	6
35	ATOM	1714	0	TYR			64.254	16.545	0.598	1.00 20.00	8
55	ATOM	1715	N	LEU			64.750	15.041	-1.001	1.00 20.00	7
	ATOM	1716	CA	LEU			65.137	13.989	-0.064	1.00 20.00	6
				LEU							6
	ATOM	1717	CB				65.283	12.649	-0.797	1.00 20.00	
40	ATOM	1718	CG	LEU			63.984	11.985	-1.274	1.00 20.00	6
40	ATOM	1719		LEU			64.314	10.802	-2.179	1.00 20.00	6
	ATOM	1720		LEU			63.160	11.530	-0.068	1.00 20.00	6
	ATOM	1721	С	LEU			66.431	14.310	0.685	1.00 20.00	6
	MOTA	1722	0	LEU	В	289	66.604	13.914	1.840	1.00 20.00	8
	ATOM	1723	N	ILE	В	290	67.340	15.017	0.025	1.00 20.00	7
45	ATOM	1724	CA	ILE	В	290	68.597	15.390	0.658	1.00 20.00	6
	ATOM	1725	СВ	ILE	В	290	69.583	15.985	-0.366	1.00 20.00	6
	ATOM	1726	CG2	ILE			70.778	16.609	0.359	1.00 20.00	6
	ATOM	1727		ILE			70.046	14.887	-1.330	1.00 20.00	6
	ATOM	1728		ILE			70.844	15.398	-2.518	1.00 20.00	6
50	ATOM	1729	C	ILE			68.307	16.424	1.743	1.00 20.00	6
50	ATOM	1730	0	ILE			68.807	16.317	2.862	1.00 20.00	8
				PHE					1.411		7
	ATOM	1731	N				67.491	17.420		1.00 20.00	
	ATOM	1732	CA	PHE			67.143	18.462	2.372	1.00 20.00	6
	ATOM	1733	СВ	PHE			66.222	19.502	1.731	1.00 20.00	6
55	ATOM	1734	CG	PHE			66.869	20.289	0.628	1.00 20.00	6
	ATOM	1735		PHE			68.255	20.420	0.568	1.00 20.00	6
	ATOM	1736	CD2	PHE	В	291	66.094	20.931	-0.332	1.00 20.00	6
	ATOM	1737	CE1	PHE	В	291	68.859	21.182	-0.435	1.00 20.00	6
	ATOM	1738		PHE			66.690	21.697	-1.340	1.00 20.00	6

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	ATOM	1739	CZ	PHE	В	291	68.074	21.822	-1.390	1.00 20.00	6
	ATOM	1740	С	PHE	В	291	66.453	17.848	3.576	1.00 20.00	6
	ATOM	1741	0	PHE	В	291	66.664	18.262	4.718	1.00 20.00	8
		1742		GLN			65.629			1.00 20.00	7
_	ATOM		N					16.847	3.303		
5	ATOM	1743	CA	GLN	В	292	64.887	16.154	4.341	1.00 20.00	6
	ATOM	1744	СВ	GLN	В	292	64.006	15.090	3.687	1.00 20.00	6
	ATOM	1745	CG	GLN	В	292	62.953	14.486	4.572	1.00 20.00	6
		1746	CD	GLN				13.750	3.763	1.00 20.00	6
	ATOM						61.895				
	ATOM	1747	OE1	GLN	В	292	62.208	12.835	2.997	1.00 20.00	8
10	ATOM	1748	NE2	GLN	В	292	60.637	14.155	3.924	1.00 20.00	7
	ATOM	1749	С	GLN	В	292	65.865	15.522	5.329	1.00 20.00	6
									6.540		8
	ATOM	1750	0	GLN			65.689	15.630		1.00 20.00	
	MOTA	1751	N	LYS	В	293	66.907	14.875	4.812	1.00 20.00	7
	ATOM	1752	CA	LYS	В	293	67.898	14.244	5.683	1.00 20.00	6
15	ATOM	1753	СВ	LYS	В	293	68.850	13.372	4.865	1.00 20.00	6
15		1754	CG	LYS				12.135		1.00 20.00	6
	ATOM						68.197		4.278		
	ATOM	1755	CD	LYS	В	293	69.217	11.260	3.554	1.00 20.00	6
	ATOM	1756	CE	LYS	В	293	68.575	9.972	3.051	1.00 20.00	6
	ATOM	1757	NZ	LYS	В	293	69.553	9.099	2.339	1.00 20.00	7
20	ATOM	1758	C	LYS			68.698	15.287	6.468	1.00 20.00	6
20											
	ATOM	1759	0	LYS			69.044	15.074	7.634	1.00 20.00	8
	ATOM	1760	N	ILE	В	294	68.989	16.411	5.827	1.00 20.00	7
	ATOM	1761	CA	ILE	В	294	69.745	17.480	6.472	1.00 20.00	6
	ATOM	1762	СВ	ILE			70.026	18.632	5.474	1.00 20.00	6
25											
25	ATOM	1763	CG2	ILE			70.489	19.881	6.223	1.00 20.00	6
	MOTA	1764	CG1	ILE	В	294	71.070	18.178	4.443	1.00 20.00	6
	ATOM	1765	CD1	ILE	В	294	71.266	19.159	3.303	1.00 20.00	6
	ATOM	1766	С	ILE			69.035	18.045	7.712	1.00 20.00	6
	ATOM	1767	0	ILE			69.618	18.091	8.798	1.00 20.00	8
30	ATOM	1768	N	ILE	В	295	67.783	18.467	7.564	1.00 20.00	7
	ATOM	1769	CA	ILE	В	295	67.068	19.037	8.707	1.00 20.00	6
	ATOM	1770	СВ	ILE			65.710	19.647	8.300	1.00 20.00	6
	MOTA	1771	CG2	ILE			65.927	20.749	7.265	1.00 20.00	6
	ATOM	1772	CG1	ILE	В	295	64.784	18.559	7.762	1.00 20.00	6
35	ATOM	1773	CD1	ILE	В	295	63.356	19.037	7.558	1.00 20.00	6
	ATOM	1774	С	ILE	В	295	66.831	18.045	9.842	1.00 20.00	6
	ATOM	1775	0	ILE			66.540	18.447	10.967	1.00 20.00	8
	MOTA	1776	N	LYS			66.956	16.753	9.550	1.00 20.00	7
	MOTA	1777	$^{\rm CA}$	LYS	В	296	66.765	15.724	10.569	1.00 20.00	6
40	ATOM	1778	СВ	LYS	В	296	65.907	14.576	10.019	1.00 20.00	6
	ATOM	1779	CG	LYS			64.535	15.010	9.538	1.00 20.00	6
	MOTA	1780	CD	LYS			63.739	13.851	8.951	1.00 20.00	6
	ATOM	1781	CE	LYS	В	296	63.296	12.873	10.025	1.00 20.00	6
	ATOM	1782	NZ	LYS	В	296	62.375	11.828	9.482	1.00 20.00	7
45	ATOM	1783	С	LYS	В	296	68.116	15.176	11.018	1.00 20.00	6
15	ATOM	1784		LYS			68.178	14.261	11.838	1.00 20.00	
			0								8
	MOTA	1785	N	LEU	В	297	69.190	15.746	10.474	1.00 20.00	7
	ATOM	1786	CA	LEU	В	297	70.551	15.320	10.791	1.00 20.00	6
	ATOM	1787	СВ	LEU	В	297	70.911	15.680	12.236	1.00 20.00	6
50	ATOM	1788	CG	LEU			72.398	15.538	12.585	1.00 20.00	6
50											
	ATOM	1789		LEU			73.215	16.555	11.771	1.00 20.00	6
	ATOM	1790	CD2	LEU	В	297	72.605	15.762	14.076	1.00 20.00	6
	ATOM	1791	С	LEU	В	297	70.635	13.810	10.592	1.00 20.00	6
	ATOM	1792	0	LEU			71.150	13.080	11.434	1.00 20.00	8
55											
55	MOTA	1793	N	GLU			70.128	13.351	9.456	1.00 20.00	7
	ATOM	1794	CA	GLU	В	298	70.115	11.934	9.148	1.00 20.00	6
	ATOM	1795	СВ	GLU	В	298	68.817	11.597	8.416	1.00 20.00	6
	ATOM	1796	CG	GLU			68.568	10.123	8.233	1.00 20.00	6
	ATOM	1797	CD	GLU	D	∠90	67.254	9.858	7.535	1.00 20.00	6

	ATOM	1798	OE1	GLU	В	298	66.214	10.331	8.043	1.00 20.00	8
	ATOM	1799	OE2	GLU	В	298	67.261	9.185	6.484	1.00 20.00	8
	ATOM	1800	С	GLU	В	298	71.309	11.446	8.332	1.00 20.00	6
	ATOM	1801	0	GLU			71.310	11.523	7.104	1.00 20.00	8
5	ATOM	1802	N	TYR			72.325	10.946	9.027	1.00 20.00	7
5											
	MOTA	1803	CA	TYR			73.519	10.405	8.390	1.00 20.00	6
	ATOM	1804	СВ	TYR	В	299	74.444	11.521	7.880	1.00 20.00	6
	MOTA	1805	CG	TYR	В	299	75.330	12.130	8.953	1.00 20.00	6
	ATOM	1806	CD1	TYR	В	299	74.796	12.962	9.935	1.00 20.00	6
10	ATOM	1807	CE1	TYR	В	299	75.589	13.482	10.951	1.00 20.00	6
	ATOM	1808		TYR			76.692	11.833	9.013	1.00 20.00	6
		1809	CE2	TYR			77.499	12.352	10.032	1.00 20.00	6
	ATOM										
	ATOM	1810	CZ	TYR			76.935	13.173	10.995	1.00 20.00	6
	MOTA	1811	OH	TYR			77.701	13.687	12.006	1.00 20.00	8
15	ATOM	1812	С	TYR	В	299	74.245	9.600	9.456	1.00 20.00	6
	ATOM	1813	0	TYR	В	299	73.913	9.688	10.631	1.00 20.00	8
	ATOM	1814	N	ASP	В	300	75.229	8.808	9.052	1.00 20.00	7
	ATOM	1815	CA	ASP	В	300	75.991	8.030	10.016	1.00 20.00	6
	ATOM	1816	СВ	ASP	В	300	75.291	6.700	10.304	1.00 20.00	6
20	ATOM	1817	CG	ASP			74.898	5.968	9.048	1.00 20.00	6
20	ATOM	1818		ASP		300	75.806	5.594	8.274	1.00 20.00	8
		1819								1.00 20.00	8
	ATOM			ASP			73.681	5.771	8.832		
	MOTA	1820	С	ASP		300	77.397	7.799	9.488	1.00 20.00	6
	ATOM	1821	0	ASP			77.651	7.976	8.297	1.00 20.00	8
25	MOTA	1822	N	PHE	В	301	78.307	7.417	10.378	1.00 20.00	7
	ATOM	1823	CA	PHE	В	301	79.695	7.186	9.996	1.00 20.00	6
	ATOM	1824	СВ	PHE	В	301	80.655	7.664	11.093	1.00 20.00	6
	ATOM	1825	CG	PHE	В	301	80.488	9.103	11.481	1.00 20.00	6
	ATOM	1826	CD1	PHE	В	301	79.493	9.487	12.370	1.00 20.00	6
30	ATOM	1827		PHE		301	81.346	10.075	10.970	1.00 20.00	6
50	ATOM	1828		PHE		301	79.352	10.823	12.750	1.00 20.00	6
		1829		PHE		301	81.214	11.408	11.342	1.00 20.00	6
	ATOM										
	ATOM	1830	CZ	PHE			80.215	11.783	12.235	1.00 20.00	6
	MOTA	1831	С	PHE		301	80.009	5.722	9.744	1.00 20.00	6
35	ATOM	1832	0	PHE		301	79.506	4.839	10.442	1.00 20.00	8
	ATOM	1833	N	PRO	В	302	80.842	5.440	8.732	1.00 20.00	7
	ATOM	1834	CD	PRO	В	302	81.330	6.316	7.654	1.00 20.00	6
	ATOM	1835	CA	PRO	В	302	81.191	4.044	8.466	1.00 20.00	6
	ATOM	1836	СВ	PRO	В	302	81.838	4.105	7.084	1.00 20.00	6
40	ATOM	1837	CG	PRO		302	82.425	5.479	7.046	1.00 20.00	6
	ATOM	1838	C	PRO		302	82.168	3.629	9.569	1.00 20.00	6
	ATOM		0	PRO			82.887			1.00 20.00	
										1.00 20.00	7
	ATOM	1840	N	ALA			82.185		9.908		
	MOTA	1841	CA	ALA			83.052	1.836		1.00 20.00	6
45	ATOM	1842	СВ	ALA			82.993	0.310	10.987	1.00 20.00	6
	ATOM	1843	С	ALA	В	303	84.513	2.294	10.939	1.00 20.00	6
	MOTA	1844	0	ALA	В	303	85.078	2.637	11.979	1.00 20.00	8
	ATOM	1845	N	ALA	В	304	85.121	2.306	9.756	1.00 20.00	7
	ATOM	1846	CA	ALA	В	304	86.527	2.684	9.605	1.00 20.00	6
50	ATOM	1847	СВ	ALA	В	304	86.971	2.423	8.165	1.00 20.00	6
	ATOM	1848	С	ALA			86.894	4.119	10.001	1.00 20.00	6
	ATOM	1849	0	ALA			87.983	4.367	10.520	1.00 20.00	8
		1850		PHE						1.00 20.00	7
	ATOM		N				85.985	5.053	9.742		
	ATOM	1851	CA	PHE			86.183	6.473	10.034	1.00 20.00	6
55	ATOM	1852	СВ	PHE			84.822	7.115	10.312	1.00 20.00	6
	MOTA	1853	CG	PHE			84.705	8.522	9.815	1.00 20.00	6
	MOTA	1854		PHE			85.303	9.572	10.502	1.00 20.00	6
	ATOM	1855	CD2	PHE	В	305		8.800	8.646	1.00 20.00	6
	ATOM	1856	CE1	PHE	В	305	85.202	10.881	10.033	1.00 20.00	6

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	ATOM	1857		PHE			83.896	10.106	8.167	1.00 20.00	6
	MOTA	1858	CZ	PHE	В	305	84.496	11.147	8.862	1.00 20.00	6
	ATOM	1859	С	PHE	В	305	87.153	6.789	11.182	1.00 20.00	6
	ATOM	1860	0	PHE	В	305	86.964	6.342	12.312	1.00 20.00	8
5	ATOM	1861	N	PHE		306	88.190	7.565	10.883	1.00 20.00	7
5						306		7.945		1.00 20.00	
	ATOM	1862	CA	PHE			89.176		11.894		6
	ATOM	1863	СВ	PHE	В	306	90.179	8.936	11.295	1.00 20.00	6
	MOTA	1864	CG	PHE	В	306	90.695	8.531	9.940	1.00 20.00	6
	ATOM	1865	CD1	PHE	В	306	91.292	7.284	9.747	1.00 20.00	6
10	ATOM	1866	CD2	PHE	В	306	90.588	9.395	8.853	1.00 20.00	6
10	ATOM	1867		PHE		306	91.774	6.906	8.490	1.00 20.00	6
	ATOM	1868		PHE		306	91.067	9.027	7.590	1.00 20.00	6
	MOTA	1869	CZ	PHE	В	306	91.662	7.780	7.408	1.00 20.00	6
	ATOM	1870	С	PHE	В	306	88.445	8.575	13.086	1.00 20.00	6
15	ATOM	1871	0	PHE	В	306	87.731	9.566	12.936	1.00 20.00	8
	ATOM	1872	N	PRO		307	88.614	7.995	14.288	1.00 20.00	7
	ATOM	1873	CD	PRO		307	89.482	6.834	14.555	1.00 20.00	6
	ATOM	1874	CA	PRO		307	87.983	8.459	15.530	1.00 20.00	6
	MOTA	1875	СВ	PRO	В	307	88.748	7.691	16.606	1.00 20.00	6
20	ATOM	1876	CG	PRO	В	307	89.018	6.388	15.928	1.00 20.00	6
	ATOM	1877	С	PRO	В	307	87.986	9.965	15.784	1.00 20.00	6
	ATOM	1878	0	PRO		307	86.936	10.565	16.025	1.00 20.00	8
	ATOM	1879	N	LYS			89.162	10.575	15.745	1.00 20.00	7
	MOTA	1880	CA	LYS	В	308	89.260	12.004	15.992	1.00 20.00	6
25	ATOM	1881	СВ	LYS	В	308	90.728	12.405	16.149	1.00 20.00	6
	ATOM	1882	CG	LYS	В	308	91.338	11.805	17.410	1.00 20.00	6
	ATOM	1883	CD	LYS			92.806	12.140	17.591	1.00 20.00	6
		1884		LYS			93.339				6
	ATOM		CE					11.457	18.847	1.00 20.00	
	ATOM	1885	NZ	LYS		308	94.816	11.573	18.985	1.00 20.00	7
30	MOTA	1886	С	LYS	В	308	88.572	12.808	14.894	1.00 20.00	6
	MOTA	1887	0	LYS	В	308	87.985	13.855	15.167	1.00 20.00	8
	ATOM	1888	N	ALA		309	88.629	12.318	13.659	1.00 20.00	7
	ATOM	1889	CA	ALA		309	87.967	13.011	12.557	1.00 20.00	6
	ATOM	1890	СВ	ALA		309	88.328	12.369	11.231	1.00 20.00	6
35	ATOM	1891	С	ALA		309	86.460	12.936	12.787	1.00 20.00	6
	ATOM	1892	0	ALA	В	309	85.735	13.903	12.552	1.00 20.00	8
	ATOM	1893	N	ARG	В	310	85.986	11.780	13.246	1.00 20.00	7
	ATOM	1894	CA	ARG	В	310	84.561	11.619	13.513	1.00 20.00	6
	ATOM	1895	СВ	ARG		310	84.246	10.194	13.979	1.00 20.00	6
40											
40	ATOM	1896	CG	ARG			82.844	10.069	14.561	1.00 20.00	6
	ATOM	1897	CD	ARG			82.408	8.632	14.789	1.00 20.00	6
	MOTA	1898	NE	ARG	В	310	81.060	8.593	15.355	1.00 20.00	7
	ATOM	1899	CZ	ARG	В	310	80.259	7.532	15.328	1.00 20.00	6
	ATOM	1900	NH1	ARG	В	310	80.665	6.401	14.759	1.00 20.00	7
45	ATOM	1901		ARG			79.048	7.601	15.867	1.00 20.00	7
15				ARG					14.583	1.00 20.00	
	ATOM	1902	С				84.110	12.613			6
	ATOM	1903	0	ARG			83.080	13.274	14.436	1.00 20.00	8
	MOTA	1904	N	ASP	В	311	84.876	12.707	15.666	1.00 20.00	7
	ATOM	1905	CA	ASP	В	311	84.535	13.629	16.740	1.00 20.00	6
50	ATOM	1906	СВ	ASP			85.574	13.555	17.864	1.00 20.00	6
	ATOM	1907	CG	ASP			85.260	14.505	19.006	1.00 20.00	6
	ATOM	1908		ASP			85.782	15.636	19.010	1.00 20.00	8
	MOTA	1909	OD2	ASP	В	311	84.480	14.124	19.901	1.00 20.00	8
	ATOM	1910	С	ASP	В	311	84.445	15.054	16.198	1.00 20.00	6
55	ATOM	1911	0	ASP			83.539	15.800	16.564	1.00 20.00	8
	ATOM	1912	N	LEU			85.371	15.423	15.313	1.00 20.00	7
		1913									
	ATOM		CA	LEU			85.362	16.769	14.736	1.00 20.00	6
	ATOM	1914	СВ	LEU			86.604	16.999	13.869	1.00 20.00	6
	ATOM	1915	CG	LEU	В	312	86.662	18.329	13.099	1.00 20.00	6

	ATOM	1916	CD1	LEU	D	312	86.424	19.510	14.037	1.00 20.00	6
	ATOM	1917		LEU		312	88.018	18.450	12.414	1.00 20.00	6
									13.899		
	ATOM	1918	С	LEU			84.112	17.008		1.00 20.00	6
-	ATOM	1919	0	LEU		312	83.456	18.039	14.035	1.00 20.00	8
5	MOTA	1920	N	VAL		313	83.786	16.051	13.033	1.00 20.00	7
	MOTA	1921	CA	VAL		313	82.611	16.171	12.183	1.00 20.00	6
	ATOM	1922	СВ	VAL			82.464	14.942	11.255	1.00 20.00	6
	MOTA	1923		VAL	В	313	81.121	14.973	10.551	1.00 20.00	6
	ATOM	1924	CG2	VAL	В	313	83.595	14.935	10.228	1.00 20.00	6
10	ATOM	1925	С	VAL	В	313	81.354	16.315	13.036	1.00 20.00	6
	ATOM	1926	0	VAL	В	313	80.467	17.111	12.716	1.00 20.00	8
	ATOM	1927	N	GLU	В	314	81.282	15.559	14.129	1.00 20.00	7
	ATOM	1928	CA	GLU	В	314	80.122	15.634	15.010	1.00 20.00	6
	ATOM	1929	СВ	GLU	В	314	80.191	14.545	16.084	1.00 20.00	6
15	ATOM	1930	CG	GLU		314	80.160	13.131	15.521	1.00 20.00	6
	ATOM	1931	CD	GLU			80.222	12.073	16.603	1.00 20.00	6
	ATOM	1932		GLU			81.033	12.227	17.542	1.00 20.00	8
	ATOM	1933		GLU			79.469	11.081	16.512	1.00 20.00	8
	ATOM	1934	C	GLU			80.035	17.005	15.664	1.00 20.00	6
20	ATOM	1935	0	GLU			78.960	17.443	16.059	1.00 20.00	8
20						315				1.00 20.00	7
	ATOM	1936	N	LYS			81.165	17.690	15.776		
	ATOM	1937	CA	LYS			81.154	19.010	16.383	1.00 20.00	6
	ATOM	1938	СВ	LYS			82.448	19.240	17.168	1.00 20.00	6
2.5	ATOM	1939	CG	LYS			82.460	18.478	18.493	1.00 20.00	6
25	ATOM	1940	CD	LYS		315	83.803	18.529	19.198	1.00 20.00	6
	ATOM	1941	CE	LYS		315	83.749	17.825	20.552	1.00 20.00	6
	ATOM	1942	NZ	LYS			82.829	18.505	21.506	1.00 20.00	7
	ATOM	1943	С	LYS		315	80.934	20.104	15.343	1.00 20.00	6
	ATOM	1944	0	LYS	В	315	80.855	21.282	15.686	1.00 20.00	8
30	ATOM	1945	N	LEU	В	316	80.819	19.706	14.075	1.00 20.00	7
	ATOM	1946	CA	LEU	В	316	80.577	20.649	12.979	1.00 20.00	6
	ATOM	1947	CB	LEU	В	316	81.608	20.450	11.863	1.00 20.00	6
	ATOM	1948	CG	LEU	В	316	83.044	20.833	12.240	1.00 20.00	6
	ATOM	1949	CD1	LEU	В	316	84.011	20.365	11.156	1.00 20.00	6
35	ATOM	1950	CD2	LEU	В	316	83.124	22.351	12.434	1.00 20.00	6
	ATOM	1951	С	LEU	В	316	79.164	20.469	12.415	1.00 20.00	6
	ATOM	1952	0	LEU			78.464	21.448	12.148	1.00 20.00	8
	ATOM	1953	N	LEU		317	78.746	19.220	12.230	1.00 20.00	7
	ATOM	1954	CA	LEU		317	77.403	18.962	11.721	1.00 20.00	6
40	ATOM	1955	СВ	LEU		317	77.343	17.605	11.012	1.00 20.00	6
.0	ATOM	1956	CG	LEU			78.335	17.445	9.852	1.00 20.00	6
	ATOM	1957		LEU			78.091	16.111	9.143	1.00 20.00	6
	ATOM	1958		LEU			78.182	18.603	8.866	1.00 20.00	6
	ATOM	1959	CDZ	LEU			76.435	19.000	12.899	1.00 20.00	6
45			0	LEU				17.966			
43	ATOM	1960					75.979		13.398	1.00 20.00	8
	ATOM	1961	N	VAL			76.156	20.215	13.354	1.00 20.00	7
	ATOM	1962	CA	VAL			75.251	20.451	14.467	1.00 20.00	6
	ATOM	1963	СВ	VAL			75.981	21.164	15.625	1.00 20.00	6
50	ATOM	1964		VAL			75.007	21.461	16.759	1.00 20.00	6
50	ATOM	1965		VAL			77.136	20.300	16.115	1.00 20.00	6
	ATOM	1966	С	VAL			74.140	21.344	13.936	1.00 20.00	6
	ATOM	1967	0	VAL			74.410	22.386	13.333	1.00 20.00	8
	ATOM	1968	N	LEU			72.892	20.941	14.153	1.00 20.00	7
	ATOM	1969	CA	LEU	В	319	71.758	21.717	13.663	1.00 20.00	6
55	ATOM	1970	СВ	LEU	В	319	70.444	21.056	14.093	1.00 20.00	6
	ATOM	1971	CG	LEU	В	319	70.211	19.647	13.533	1.00 20.00	6
	ATOM	1972	CD1	LEU			68.883	19.098	14.060	1.00 20.00	6
	ATOM	1973		LEU			70.211	19.688	12.000	1.00 20.00	6
	ATOM	1974	С	LEU			71.794	23.173	14.119	1.00 20.00	6

	ATOM	1975	0	LEU	В	319	71.591	24.082	13.317	1.00	20.00	8
	ATOM	1976	N	ASP			72.052	23.394	15.405		20.00	7
	ATOM	1977	CA	ASP			72.119	24.745	15.958		20.00	6
	ATOM	1978	CB	ASP			72.091	24.687	17.490		20.00	6
5	ATOM	1979	CG	ASP		320	72.058	26.061	18.129		20.00	6
,	ATOM	1980		ASP			72.506	27.036	17.492		20.00	8
	ATOM	1981		ASP			71.595	26.166	19.284		20.00	8
	ATOM	1982	C	ASP			73.415	25.419	15.492		20.00	6
	ATOM	1983	0	ASP			74.496	25.089	15.965		20.00	8
10	ATOM	1984	N	ALA			73.294	26.372	14.576		20.00	7
	ATOM	1985	CA	ALA			74.450	27.078	14.028		20.00	6
	ATOM	1986	СВ	ALA			73.982	28.109	13.006		20.00	6
	ATOM	1987	C	ALA			75.359	27.747	15.065		20.00	6
	ATOM	1988	0	ALA			76.535	27.992	14.790		20.00	8
15	ATOM	1989	N	THR			74.829	28.035	16.252		20.00	7
10	ATOM	1990	CA	THR			75.631	28.681	17.292		20.00	6
	ATOM	1991	СВ	THR			74.755	29.491	18.271		20.00	6
	ATOM	1992		THR		322	73.879	28.605	18.973		20.00	8
	ATOM	1993		THR			73.928	30.527	17.519		20.00	6
20	ATOM	1994	C	THR			76.437	27.684	18.108		20.00	6
	ATOM	1995	0	THR			77.166	28.071	19.019		20.00	8
	ATOM	1996	N	LYS			76.312	26.401	17.786		20.00	7
	ATOM	1997	CA	LYS		323	77.048	25.378	18.517		20.00	6
	ATOM	1998	CB	LYS			76.080	24.378	19.155		20.00	6
25	ATOM	1999	CG	LYS			75.180	24.992	20.209		20.00	6
	ATOM	2000	CD	LYS			74.356	23.931	20.924		20.00	6
	ATOM	2001	CE	LYS			73.406	24.574	21.927		20.00	6
	ATOM	2002	NZ	LYS			74.144	25.514	22.818		20.00	7
	ATOM	2003	C	LYS			78.066	24.631	17.664		20.00	6
30	ATOM	2004	0	LYS		323	78.520	23.557	18.040		20.00	8
50	ATOM	2005	N	ARG		324	78.427	25.195	16.517		20.00	7
	ATOM	2006	CA	ARG		324	79.408	24.545	15.656		20.00	6
	ATOM	2007	СВ	ARG		324	79.108	24.834	14.186		20.00	6
	ATOM	2008	CG	ARG		324	77.824	24.177	13.728		20.00	6
35	ATOM	2009	CD	ARG		324	77.468	24.505	12.297		20.00	6
	ATOM	2010	NE	ARG		324	76.060	24.202	12.069		20.00	7
	ATOM	2011	CZ	ARG			75.277	24.873	11.233		20.00	6
	ATOM	2012		ARG			75.764	25.888	10.523		20.00	7
	ATOM	2013		ARG			73.992	24.551	11.140		20.00	7
40	ATOM	2014	С	ARG		324	80.811	25.011	16.008		20.00	6
	ATOM	2015	0	ARG			81.070	26.212	16.131		20.00	8
	ATOM		N	LEU				24.049				
	ATOM	2017	CA	LEU			83.090	24.350	16.520		20.00	6
	ATOM	2018	СВ	LEU			83.913		16.550		20.00	6
45	ATOM	2019	CG	LEU			85.274	23.123	17.241		20.00	6
	MOTA	2020		LEU			85.093	23.591	18.682		20.00	6
	ATOM	2021		LEU			85.922	21.741	17.209		20.00	6
	ATOM	2022	С	LEU			83.656	25.310	15.481		20.00	6
	ATOM	2023	0	LEU			83.649	25.015	14.282		20.00	8
50	ATOM	2024	N	GLY			84.139	26.461	15.946		20.00	7
	MOTA	2025	CA	GLY			84.697	27.449	15.040		20.00	6
	ATOM	2026	С	GLY			83.857	28.711	14.932		20.00	6
	MOTA	2027	0	GLY			84.369	29.757	14.529		20.00	8
	ATOM	2028	N	CYS			82.575	28.632	15.286		20.00	7
55	ATOM	2029	CA	CYS			81.714	29.806	15.200		20.00	6
	ATOM	2030	CB	CYS			80.233	29.404	15.183		20.00	6
	ATOM	2030	SG	CYS			79.534	28.915	16.774		20.00	
	ATOM	2032	C	CYS			81.976	30.772	16.353		20.00	6
	ATOM	2032	0	CYS			82.565	30.410	17.371		20.00	8
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	ATOM	2034	N	GLU	В	328	81.523	32.005	16.178	1.00	20.00	7
	ATOM	2035	CA	GLU		328	81.714	33.052	17.167		20.00	6
	ATOM	2036	СВ	GLU		328	81.087	34.348	16.632		20.00	6
	ATOM	2037	CG	GLU		328	81.734	34.772	15.300		20.00	6
5	ATOM	2038	CD	GLU		328	80.962	35.842	14.539		20.00	6
5	ATOM	2039		GLU		328	79.738	35.676	14.343		20.00	8
	ATOM	2040	OE2	GLU			81.588	36.840	14.116		20.00	8
	ATOM	2040	C	GLU		328	81.187	32.701	18.560		20.00	6
		2041	0	GLU			81.850	32.701	19.562		20.00	8
10	ATOM	2042		GLU			80.016	32.903	18.631		20.00	7
10	ATOM		N									
	ATOM	2044	CA	GLU		329	79.449	31.714	19.926		20.00	6
	ATOM	2045	СВ	GLU			77.991	31.263	19.782		20.00	6
	ATOM	2046	CG	GLU		329	77.028	32.355	19.315		20.00	6
1.5	ATOM	2047	CD	GLU			77.055	32.575	17.813		20.00	6
15	ATOM	2048		GLU		329	77.859	31.910	17.120		20.00	8
	ATOM	2049	OE2	GLU		329	76.267	33.413	17.323		20.00	8
	MOTA	2050	С	GLU			80.264	30.616	20.605		20.00	6
	ATOM	2051	0	GLU			80.182	30.436	21.819		20.00	8
	ATOM	2052	N	MET			81.040	29.878	19.816		20.00	7
20	ATOM	2053	CA	MET			81.880	28.813	20.354		20.00	6
	ATOM	2054	СВ	MET		330	81.872	27.600	19.419		20.00	6
	MOTA	2055	CG	MET	В	330	80.552	26.822	19.436	1.00	20.00	6
	ATOM	2056	SD	MET	В	330	80.117	26.254	21.104	1.00	20.00	16
	ATOM	2057	CE	MET	В	330	81.265	24.895	21.311	1.00	20.00	6
25	ATOM	2058	С	MET	В	330	83.302	29.330	20.547	1.00	20.00	6
	ATOM	2059	0	MET	В	330	84.236	28.564	20.754	1.00	20.00	8
	ATOM	2060	N	GLU	В	331	83.443	30.647	20.471	1.00	20.00	7
	ATOM	2061	CA	GLU	В	331	84.716	31.338	20.656	1.00	20.00	6
	ATOM	2062	СВ	GLU	В	331	85.357	30.921	21.987	1.00	20.00	6
30	ATOM	2063	CG	GLU	В	331	84.371	30.886	23.163	1.00	20.00	6
	ATOM	2064	CD	GLU	В	331	83.478	32.127	23.270	1.00	20.00	6
	ATOM	2065	OE1	GLU	В	331	82.483	32.064	24.021	1.00	20.00	8
	ATOM	2066	OE2	GLU		331	83.759	33.159	22.625		20.00	8
	ATOM	2067	С	GLU	В	331	85.742	31.247	19.523	1.00	20.00	6
35	ATOM	2068	0	GLU	В	331	86.952	31.264	19.761	1.00	20.00	8
	ATOM	2069	N	GLY			85.257	31.137	18.292		20.00	7
	ATOM	2070	CA	GLY			86.145	31.159	17.140		20.00	6
	ATOM	2071	С	GLY			87.036	30.014	16.721		20.00	6
	ATOM	2072	0	GLY			86.881	28.863	17.142		20.00	8
40	ATOM	2073	N	TYR			88.002	30.366	15.875		20.00	7
	ATOM	2074	CA	TYR			88.939	29.413	15.307		20.00	6
	ATOM	2075	СВ	TYR			89.625	30.053	14.093		20.00	6
	ATOM	2076	CG	TYR			88.724	30.031	12.877		20.00	6
	ATOM	2077		TYR			88.774	28.966	11.974		20.00	6
45	ATOM	2078		TYR			87.872	28.869	10.919		20.00	6
15	ATOM	2079		TYR			87.747	31.011	12.686		20.00	6
	ATOM	2080		TYR			86.831	30.923	11.624		20.00	6
	ATOM	2081	CZ	TYR			86.903	29.845	10.751		20.00	6
	ATOM	2082	OH	TYR			86.001	29.719	9.724		20.00	8
50	ATOM	2082	C	TYR			89.958	28.800	16.252		20.00	
50		2083		TYR					15.971		20.00	6
	ATOM		O				90.473	27.721				8
	ATOM	2085	N	GLY			90.242	29.469	17.369		20.00	7
	ATOM	2086	CA	GLY			91.193	28.921	18.327		20.00	6
55	ATOM	2087	C	GLY			90.803	27.504	18.741		20.00	6
55	ATOM	2088	0	GLY			91.577	26.564	18.558		20.00	8
	ATOM	2089	N	PRO			89.603	27.320	19.309		20.00	7
	ATOM	2090	CD	PRO			88.703	28.372	19.814		20.00	6
	ATOM	2091	CA	PRO			89.145	25.991	19.731		20.00	6
	ATOM	2092	СВ	PRO	В	335	87.759	26.275	20.303	1.00	20.00	6

	ATOM	2093	CG	PRO	B	335	87.925	27.644	20.883	1.00 20.00	6
	ATOM	2093		PRO		335	89.104	24.986	18.573	1.00 20.00	6
			С								
	ATOM	2095	0	PRO			89.406	23.808	18.756	1.00 20.00	8
-	ATOM	2096	N	LEU		336	88.727	25.450	17.382	1.00 20.00	7
5	MOTA	2097	CA	LEU		336	88.666	24.567	16.219	1.00 20.00	6
	MOTA	2098	СВ	LEU		336	88.031	25.292	15.023	1.00 20.00	6
	ATOM	2099	CG	LEU			88.051	24.581	13.663	1.00 20.00	6
	MOTA	2100	CD1	LEU	В	336	87.486	23.177	13.787	1.00 20.00	6
	MOTA	2101	CD2	LEU	В	336	87.239	25.399	12.653	1.00 20.00	6
10	ATOM	2102	С	LEU	В	336	90.060	24.068	15.839	1.00 20.00	6
	ATOM	2103	0	LEU	В	336	90.274	22.870	15.665	1.00 20.00	8
	ATOM	2104	N	LYS	В	337	91.011	24.986	15.717	1.00 20.00	7
	ATOM	2105	CA	LYS	В	337	92.370	24.597	15.360	1.00 20.00	6
	ATOM	2106	СВ	LYS		337	93.198	25.848	15.046	1.00 20.00	6
15	ATOM	2107	CG	LYS			92.678	26.560	13.801	1.00 20.00	6
	ATOM	2108	CD	LYS			93.111	28.014	13.717	1.00 20.00	6
	ATOM	2109	CE	LYS			94.561	28.167	13.314	1.00 20.00	6
	ATOM	2110	ΝZ	LYS			94.882	29.611	13.122	1.00 20.00	7
	ATOM	2111	C	LYS			93.020	23.764	16.467	1.00 20.00	6
20	ATOM	2112	0	LYS			93.965	23.704	16.215	1.00 20.00	8
20						338	92.495			1.00 20.00	7
	ATOM	2113	N	ALA				23.866	17.684		
	ATOM	2114	CA	ALA			93.056	23.105	18.799	1.00 20.00	6
	ATOM	2115	СB	ALA			92.873	23.877	20.105	1.00 20.00	6
2.5	ATOM	2116	С	ALA			92.441	21.718	18.929	1.00 20.00	6
25	ATOM	2117	0	ALA			92.805	20.955	19.820	1.00 20.00	8
	ATOM	2118	N	HIS		339	91.513	21.375	18.043	1.00 20.00	7
	ATOM	2119	CA	HIS			90.886	20.061	18.129	1.00 20.00	6
	ATOM	2120	СВ	HIS			89.786	19.919	17.074	1.00 20.00	6
	ATOM	2121	CG	HIS		339	88.999	18.654	17.199	1.00 20.00	6
30	ATOM	2122	CD2	HIS		339	87.797	18.406	17.774	1.00 20.00	6
	MOTA	2123	ND1	HIS	В	339	89.462	17.440	16.737	1.00 20.00	7
	ATOM	2124	CE1	HIS	В	339	88.578	16.498	17.021	1.00 20.00	6
	ATOM	2125	NE2	HIS	В	339	87.559	17.057	17.650	1.00 20.00	7
	ATOM	2126	С	HIS	В	339	91.928	18.952	17.970	1.00 20.00	6
35	ATOM	2127	0	HIS	В	339	92.863	19.077	17.186	1.00 20.00	8
	ATOM	2128	N	PRO	В	340	91.780	17.854	18.731	1.00 20.00	7
	ATOM	2129	CD	PRO	В	340	90.747	17.655	19.765	1.00 20.00	6
	ATOM	2130	CA	PRO	В	340	92.700	16.711	18.694	1.00 20.00	6
	ATOM	2131	СВ	PRO		340	91.966	15.665	19.521	1.00 20.00	6
40	ATOM	2132	CG	PRO		340	91.310	16.505	20.579	1.00 20.00	6
	ATOM	2133	C	PRO			93.072	16.198	17.301	1.00 20.00	6
	ATOM	2134	0	PRO			94.193	15.748	17.080	1.00 20.00	8
	ATOM	2135	N	PHE			92.139	16.270	16.362	1.00 20.00	7
	ATOM	2136	CA	PHE			92.407	15.797	15.011	1.00 20.00	6
45	ATOM	2137	CB	PHE			91.152	15.943	14.142	1.00 20.00	6
73	ATOM	2138	CG	PHE			91.317	15.424		1.00 20.00	
				PHE					12.738		6
	ATOM	2139					91.596	14.080	12.507	1.00 20.00	6
	ATOM	2140		PHE			91.182	16.277	11.647	1.00 20.00	6
50	ATOM	2141		PHE			91.738	13.592	11.207	1.00 20.00	6
50	ATOM	2142		PHE			91.320	15.803	10.345	1.00 20.00	6
	ATOM	2143	CZ	PHE			91.599	14.457	10.123	1.00 20.00	6
	MOTA	2144	С	PHE			93.571	16.550	14.362	1.00 20.00	6
	ATOM	2145	0	PHE			94.268	16.002	13.514	1.00 20.00	8
	ATOM	2146	N	PHE			93.777	17.800	14.765	1.00 20.00	7
55	ATOM	2147	CA	PHE			94.842	18.630	14.202	1.00 20.00	6
	MOTA	2148	СВ	PHE	В	342	94.336	20.058	13.975	1.00 20.00	6
	ATOM	2149	CG	PHE	В	342	93.124	20.152	13.096	1.00 20.00	6
	ATOM	2150	CD1	PHE	В	342	93.166	19.729	11.777	1.00 20.00	6
	ATOM	2151		PHE			91.954	20.734	13.575	1.00 20.00	6

	7. [] () (0150	CE1	PHE	ъ	242	02 050	10 000	10 026	1 00 20 00	c
	ATOM	2152					92.058	19.888	10.936	1.00 20.00	6
	ATOM	2153	CE2	PHE		342	90.843	20.898	12.742	1.00 20.00	6
	ATOM	2154	CZ	PHE			90.898	20.475	11.423	1.00 20.00	6
	ATOM	2155	С	PHE		342	96.077	18.718	15.101	1.00 20.00	6
5	MOTA	2156	0	PHE	В	342	96.932	19.584	14.902	1.00 20.00	8
	MOTA	2157	N	GLU	В	343	96.173	17.829	16.083	1.00 20.00	7
	MOTA	2158	CA	GLU	В	343	97.293	17.857	17.022	1.00 20.00	6
	ATOM	2159	СВ	GLU	В	343	97.330	16.564	17.841	1.00 20.00	6
	ATOM	2160	CG	GLU			98.475	16.525	18.839	1.00 20.00	6
10	ATOM	2161	CD	GLU			98.372	15.365	19.813	1.00 20.00	6
10	ATOM	2162		GLU		343	98.290	14.201	19.359	1.00 20.00	8
											8
	ATOM	2163	OE2	GLU			98.379	15.622	21.036	1.00 20.00	
	ATOM	2164	С	GLU		343	98.683	18.113	16.430	1.00 20.00	6
	ATOM	2165	0	GLU			99.419	18.969	16.925	1.00 20.00	8
15	ATOM	2166	N	SER			99.047	17.382	15.383	1.00 20.00	7
	MOTA	2167	CA	SER	В	344	100.370	17.549	14.781	1.00 20.00	6
	MOTA	2168	СВ	SER	В	344	100.848	16.219	14.192	1.00 20.00	6
	MOTA	2169	OG	SER	В	344	100.072	15.856	13.065	1.00 20.00	8
	ATOM	2170	С	SER	В	344	100.467	18.629	13.702	1.00 20.00	6
20	ATOM	2171	0	SER	В	344	101.485	18.732	13.025	1.00 20.00	8
	ATOM	2172	N	VAL		345	99.423	19.435	13.544	1.00 20.00	7
	ATOM	2173	CA	VAL		345	99.430	20.486	12.527	1.00 20.00	6
		2174	CB	VAL			97.985	20.843	12.075	1.00 20.00	6
	ATOM										
25	ATOM	2175		VAL			98.015	22.042	11.120	1.00 20.00	6
25	ATOM	2176		VAL			97.335	19.646	11.400	1.00 20.00	6
	ATOM	2177	С	VAL		345	100.096	21.785	12.980	1.00 20.00	6
	ATOM	2178	0	VAL	В	345	99.844	22.275	14.085	1.00 20.00	8
	ATOM	2179	N	THR	В	346	100.951	22.335	12.122	1.00 20.00	7
	ATOM	2180	CA	THR	В	346	101.602	23.610	12.397	1.00 20.00	6
30	ATOM	2181	СВ	THR	В	346	103.096	23.593	11.982	1.00 20.00	6
	ATOM	2182	OG1	THR	В	346	103.816	22.688	12.831	1.00 20.00	8
	ATOM	2183	CG2	THR	В	346	103.707	24.983	12.115	1.00 20.00	6
	ATOM	2184	С	THR		346	100.810	24.573	11.510	1.00 20.00	6
	ATOM	2185	0	THR		346	100.950	24.565	10.285	1.00 20.00	8
35	ATOM	2186	N	TRP		347	99.966	25.385	12.138	1.00 20.00	7
33	ATOM	2187	CA	TRP		347	99.089	26.306	11.425	1.00 20.00	6
	ATOM	2188	CB	TRP			97.941	26.727	12.344	1.00 20.00	6
	ATOM	2189	CG	TRP		347	97.088	25.594	12.818	1.00 20.00	6
4.0	ATOM	2190	CD2	TRP		347	95.924	25.071	12.165	1.00 20.00	6
40	ATOM	2191	CE2			347	95.436	24.008	12.963	1.00 20.00	6
	ATOM	2192	CE3	TRP			95.247	25.397	10.983	1.00 20.00	6
	MOTA	2193	CD1	TRP	В	347	97.259	24.848	13.953	1.00 20.00	6
	ATOM	2194	NE1	TRP	В	347	96.269	23.893	14.048	1.00 20.00	7
	MOTA	2195	CZ2	TRP	В	347	94.300	23.270	12.616	1.00 20.00	6
45	MOTA	2196	CZ3	TRP	В	347	94.113	24.661	10.636	1.00 20.00	6
	ATOM	2197		TRP			93.654	23.610	11.452	1.00 20.00	6
	ATOM	2198	С	TRP			99.679	27.563	10.800	1.00 20.00	6
	ATOM	2199	0	TRP			99.101	28.114	9.867	1.00 20.00	8
	ATOM	2200	N	ALA			100.820	28.016	11.308	1.00 20.00	7
50	ATOM	2201	CA	ALA			101.439	29.247	10.822	1.00 20.00	6
50	ATOM	2202	CB	ALA						1.00 20.00	
							102.582	29.656	11.761		6
	ATOM	2203	С	ALA			101.933	29.277	9.381	1.00 20.00	6
	ATOM	2204	0	ALA			101.874	30.323	8.738	1.00 20.00	8
	ATOM	2205	N	ASN			102.411	28.152	8.860	1.00 20.00	7
55	ATOM	2206	CA	ASN			102.940	28.153	7.500	1.00 20.00	6
	ATOM	2207	СВ	ASN	В	349	104.466	28.205	7.569	1.00 20.00	6
	ATOM	2208	CG	ASN	В	349	105.058	26.929	8.138	1.00 20.00	6
	ATOM	2209	OD1	ASN	В	349	104.445	26.282	8.984	1.00 20.00	8
	ATOM	2210		ASN			106.251	26.563	7.678	1.00 20.00	7

	ATOM	2211	С	ASN	D	240	102.522	26.966	6.634	1.00 20.00	6
	ATOM	2212		ASN		349	102.322	26.371	5.944	1.00 20.00	8
			0								
	ATOM	2213	N	LEU			101.242	26.628	6.643	1.00 20.00	7
_	ATOM	2214	CA	LEU		350	100.776	25.500	5.846	1.00 20.00	6
5	MOTA	2215	СВ	LEU		350	99.257	25.355	5.973	1.00 20.00	6
	MOTA	2216	CG	LEU	В	350	98.734	24.848	7.316	1.00 20.00	6
	ATOM	2217	CD1	LEU	В	350	97.244	25.127	7.418	1.00 20.00	6
	MOTA	2218	CD2	LEU	В	350	99.030	23.357	7.444	1.00 20.00	6
	MOTA	2219	С	LEU	В	350	101.147	25.574	4.365	1.00 20.00	6
10	ATOM	2220	0	LEU	В	350	101.557	24.575	3.775	1.00 20.00	8
	MOTA	2221	N	HIS	В	351	101.006	26.744	3.752	1.00 20.00	7
	MOTA	2222	CA	HIS	В	351	101.305	26.829	2.329	1.00 20.00	6
	MOTA	2223	СВ	HIS			100.651	28.087	1.721	1.00 20.00	6
	ATOM	2224	CG	HIS			101.553	29.274	1.618	1.00 20.00	6
15	ATOM	2225		HIS			102.001	30.143	2.556	1.00 20.00	6
15	ATOM	2226		HIS			102.072	29.706	0.416	1.00 20.00	7
	ATOM	2227		HIS			102.798	30.792	0.618	1.00 20.00	6
				HIS			102.730		1.907	1.00 20.00	7
	ATOM	2228						31.079			
20	ATOM	2229	C	HIS			102.797	26.731	1.999	1.00 20.00	6
20	ATOM	2230	0	HIS			103.176	26.669	0.832	1.00 20.00	8
	ATOM	2231	N	GLN		352	103.634	26.685	3.033	1.00 20.00	7
	MOTA	2232	CA	GLN			105.081	26.554	2.851	1.00 20.00	6
	MOTA	2233	СВ	GLN			105.841	27.458	3.819	1.00 20.00	6
	ATOM	2234	CG	GLN			106.395	28.705	3.166	1.00 20.00	6
25	MOTA	2235	CD	GLN	В	352	105.930	29.966	3.854	1.00 20.00	6
	MOTA	2236	OE1	GLN		352	106.134	30.139	5.053	1.00 20.00	8
	ATOM	2237	NE2	GLN	В	352	105.299	30.854	3.096	1.00 20.00	7
	MOTA	2238	С	GLN	В	352	105.478	25.099	3.088	1.00 20.00	6
	ATOM	2239	0	GLN	В	352	106.632	24.715	2.895	1.00 20.00	8
30	ATOM	2240	N	GLN	В	353	104.514	24.295	3.522	1.00 20.00	7
	ATOM	2241	CA	GLN		353	104.761	22.888	3.777	1.00 20.00	6
	ATOM	2242	СВ	GLN			103.849	22.395	4.900	1.00 20.00	6
	ATOM	2243	CG	GLN		353	104.122	23.050	6.240	1.00 20.00	6
	ATOM	2244	CD	GLN		353	103.075	22.711	7.281	1.00 20.00	6
35	ATOM	2245		GLN		353	102.627	21.571	7.377	1.00 20.00	8
33	ATOM	2246	NE2	GLN			102.690	23.700	8.076	1.00 20.00	7
	ATOM	2247	C	GLN			104.507	22.079	2.510	1.00 20.00	6
		2247	0	GLN			104.307	22.490	1.641	1.00 20.00	8
	ATOM	2249				354				1.00 20.00	7
40	ATOM		N	THR THR			105.172	20.937	2.401		
40	ATOM	2250	CA				104.998		1.244	1.00 20.00	6
	ATOM	2251	CB	THR			106.240	19.173	1.029	1.00 20.00	6
	ATOM	2252	OG1				107.390	19.999	0.790	1.00 20.00	8
	ATOM	2253		THR			106.033	18.243	-0.166	1.00 20.00	6
4.5	ATOM	2254	С	THR			103.777	19.197	1.501	1.00 20.00	6
45	MOTA	2255	0	THR			103.745	18.426	2.454	1.00 20.00	8
	MOTA	2256	N	PRO			102.741	19.319	0.658	1.00 20.00	7
	MOTA	2257	CD	PRO			102.547	20.275	-0.444	1.00 20.00	6
	MOTA	2258	CA	PRO			101.540	18.505	0.859	1.00 20.00	6
	MOTA	2259	СВ	PRO			100.616	18.967	-0.266	1.00 20.00	6
50	MOTA	2260	CG	PRO	В	355	101.039	20.387	-0.490	1.00 20.00	6
	MOTA	2261	С	PRO	В	355	101.835	17.011	0.766	1.00 20.00	6
	MOTA	2262	0	PRO	В	355	102.631	16.577	-0.065	1.00 20.00	8
	ATOM	2263	N	PRO	В	356	101.198	16.204	1.625	1.00 20.00	7
	MOTA	2264	CD	PRO			100.128	16.522	2.587	1.00 20.00	6
55	ATOM	2265	CA	PRO			101.438	14.761	1.573	1.00 20.00	6
	ATOM	2266	СВ	PRO			100.593	14.235	2.729	1.00 20.00	6
	ATOM	2267	CG	PRO			99.429	15.188	2.723	1.00 20.00	6
	ATOM	2268	C	PRO			100.960	14.244	0.222	1.00 20.00	6
			0				100.900			1.00 20.00	8
	ATOM	2269	U	PRO	Ď	226	100.003	14.779	-0.346	1.00 20.00	0

	ATOM	2270	N	ALA	В	357	101.629	13.221	-0.300	1.00 20.0	0 7	
	ATOM	2271	CA	ALA	В	357	101.247	12.660	-1.588	1.00 20.0	0 6	
	ATOM	2272	СВ	ALA	В	357	102.352	11.750	-2.118	1.00 20.0	0 6	
	ATOM	2273	С	ALA	В	357	99.948	11.883	-1.427	1.00 20.0	0 6	
5	ATOM	2274	0	ALA	В	357	99.808	11.074	-0.506	1.00 20.0	0 8	
	ATOM	2275	N	LEU	В	358	99.000	12.134	-2.323	1.00 20.0		
	ATOM	2276	CA	LEU			97.709	11.460	-2.278	1.00 20.0		
	ATOM	2277	СВ	LEU			96.729	12.166	-3.217	1.00 20.0		
	ATOM	2278	CG			358	96.368	13.582	-2.766	1.00 20.0		
10	ATOM	2279		LEU			95.513	14.262	-3.813	1.00 20.0		
10	ATOM	2280		LEU			95.636	13.516	-1.430	1.00 20.0		
		2281	CDZ	LEU			97.813	9.976	-2.633	1.00 20.0		
	ATOM			LEU						1.00 20.0		
	ATOM	2282	0				97.918	9.614	-3.806			
1.5	ATOM	2283	N			359	97.776	9.134	-1.600	1.00 20.0		
15	ATOM	2284	CA	THR		359	97.867	7.678	-1.735	1.00 20.0		
	ATOM	2285	СВ	THR			96.513	7.046	-2.149	1.00 20.0		
	ATOM	2286		THR			96.111	7.555	-3.427	1.00 20.0		
	ATOM	2287	CG2	THR			95.439	7.355	-1.112	1.00 20.0		
	ATOM	2288	С			359	98.933	7.238	-2.736	1.00 20.0		
20	ATOM	2289	0	THR	В	359	99.903	7.998	-2.945	1.00 20.0		
	ATOM	2290	OXT	THR	В	359	98.802	6.121	-3.280	1.00 20.0	0 8	
	TER											
	ATOM	2291	OH2	TIP	S	1	42.566	19.118	34.302	1.00 15.0	9	S
	ATOM	2292	OH2	TIP	S	2	41.052	32.378	19.857	1.00 15.8	2	S
25	ATOM	2293	OH2	TIP	S	3	37.014	33.030	17.747	1.00 16.9	5	S
	ATOM	2294	OH2	TIP	S	5	45.353	24.370	18.152	1.00 16.8	5	S
	ATOM	2295	OH2			6	31.896	13.930	33.235	1.00 20.4	2	S
	ATOM	2296	OH2			7	50.351	22.781	28.249	1.00 21.1		S
	ATOM	2297			S	8	45.246	-0.589	-0.734	1.00 17.7		S
30	ATOM	2298		TIP		11	46.249	-0.348	-8.523	1.00 21.3		S
50	ATOM	2299			S	14	45.756	11.148	29.680	1.00 21.9		S
	ATOM	2300		TIP		15	44.273	13.157	34.592	1.00 21.5		S
		2300	OH2			17	53.598	3.722		1.00 13.8		S
	ATOM								-1.720			
25	ATOM	2302		TIP		18	46.049	13.087	31.565	1.00 20.3		S
35	ATOM	2303		TIP		19	53.422	22.401	-3.280	1.00 23.2		S
	ATOM	2304	OH2		S	20	34.587	7.922	5.383	1.00 22.5		S
	ATOM	2305	OH2			21	45.053	27.379	19.376	1.00 29.6		S
	ATOM	2306			S	23	28.899	36.416	28.633	1.00 31.6		S
4.0	ATOM	2307		TIP		24	35.531	11.645	-8.219	1.00 23.4		S
40	ATOM	2308		TIP		25	47.364	28.787	19.612	1.00 23.0		S
	ATOM	2309		TIP		27	48.859	21.588	12.634	1.00 23.7		S
	MOTA	2310						8.920		1.00 22.2		S
	MOTA	2311	OH2	TIP	S	31	48.619	7.247	10.112	1.00 21.3		S
	ATOM	2312	OH2	TIP	S	34	44.824	28.720	15.621	1.00 25.2	7	S
45	MOTA	2313	OH2	TIP	S	35	26.030	12.634	13.407	1.00 21.6	1	S
	ATOM	2314	OH2	TIP	S	36	50.462	19.810	40.066	1.00 25.4	5	S
	ATOM	2315	OH2	TIP	S	37	39.631	23.510	-0.239	1.00 30.8	8	S
	ATOM	2316	OH2	TIP	S	40	44.734	42.655	10.346	1.00 30.8	4	S
	ATOM	2317	OH2	TIP	S	41	54.653	3.902	1.503	1.00 27.1	4	S
50	ATOM	2318		TIP		45	45.693	21.923	39.754	1.00 28.3	0	S
	ATOM	2319		TIP		47	47.820	16.413	7.805	1.00 25.7		S
	ATOM	2320		TIP		48	50.292	31.412	29.642	1.00 32.7		S
	ATOM	2321		TIP		49	26.056	16.646	34.827	1.00 29.8		S
	ATOM	2322		TIP		52	31.714	10.040	31.855	1.00 29.1		S
55	ATOM	2323		TIP		53	46.108	23.843	-4.299	1.00 29.1		s S
ננ												
	ATOM	2324		TIP		54	37.645	11.206	34.448	1.00 28.5		S
	MOTA	2325		TIP		55 50	26.371	28.513	12.142	1.00 32.0		S
	ATOM	2326		TIP		58	33.564	19.700	3.483	1.00 28.2		S
	ATOM	2327	OH2	TIP	S	64	48.295	-0.632	14.280	1.00 32.1	3	S

			_							
	MOTA	2328	OH2	TIP S	65	40.064	26.036	34.324	1.00 24.17	S
	MOTA	2329	OH2 '	TIP S	66	29.570	3.958	14.729	1.00 28.94	S
	ATOM	2330	ОН2	TIP S	72	60.085	11.604	6.814	1.00 38.35	S
		2331	OH2 '			39.203	44.403	18.686		
_	ATOM								1.00 26.61	S
5	MOTA	2332	OH2	TIP S	76	47.312	12.366	27.366	1.00 28.51	S
	MOTA	2333	OH2 '	TIP S	80	43.862	33.771	33.329	1.00 28.82	S
	ATOM	2334	он2 :	TIP S	81	57.890	13.106	2.128	1.00 40.62	S
		2335		TIP S			34.381	32.043	1.00 19.35	S
	ATOM					41.663				
	ATOM	2336	OH2	TIP S	85	50.974	40.331	19.200	1.00 21.14	S
10	ATOM	2337	OH2 !	TIP S	88	47.925	-0.832	-6.556	1.00 24.11	S
	ATOM	2338	он2 !	TIP S	90	27.231	28.336	33.481	1.00 27.64	S
	ATOM	2339	OH2 '			43.651	-7.101	-7.995	1.00 24.33	S
	ATOM	2340	OH2			49.325	4.387	19.370	1.00 28.02	S
	MOTA	2341	OH2	TIP S	93	46.231	11.549	33.898	1.00 29.40	S
15	ATOM	2342	OH2 '	TIP S	94	63.889	24.831	1.168	1.00 26.53	S
	ATOM	2343	OH2 '	TIP S	96	56.396	4.952	-6.749	1.00 28.00	S
	ATOM	2344		TIP S		35.510	27.986	11.558	1.00 29.24	S
	ATOM	2345	OH2 !	LIB 8	3 100	49.942	24.366	30.265	1.00 31.61	S
	MOTA	2346	OH2 '	TIP S	101	56.121	7.113	-8.298	1.00 31.57	S
20	ATOM	2347	OH2 '	TIP S	102	58.318	19.957	-8.378	1.00 26.95	S
	ATOM	2348			103	49.647	22.446	39.624	1.00 40.57	S
	ATOM	2349	OH2 '			45.359	7.052	13.052	1.00 26.27	S
	ATOM	2350	OH2 !			37.150	32.340	32.346	1.00 34.45	S
	MOTA	2351	OH2 !	TIP S	107	43.465	40.457	8.240	1.00 40.48	S
25	ATOM	2352	OH2 '	TIP S	119	36.644	8.257	13.418	1.00 30.70	S
	ATOM	2353		TIP S		41.912	-8.974	-8.264	1.00 26.08	S
									1.00 24.08	
	ATOM	2354		TIP S		62.424	15.800	-7.411		S
	ATOM	2355	OH2	rip s	126	37.266	18.656	-9.097	1.00 28.99	S
	MOTA	2356	OH2	TIP S	127	43.129	26.845	14.606	1.00 25.19	S
30	ATOM	2357	OH2 '	TIP S	128	36.339	32.639	29.802	1.00 29.25	S
	ATOM	2358		TIP S		54.051	14.561	26.498	1.00 33.93	S
	ATOM	2359		TIP S		41.805	-4.242	5.492	1.00 33.72	S
	MOTA	2360		TIP S		38.873	25.163	36.697	1.00 30.69	S
	MOTA	2361	OH2	TIP S	134	28.777	8.553	25.307	1.00 31.43	S
35	ATOM	2362	OH2 '	TIP S	135	53.672	10.546	-12.803	1.00 33.45	S
	ATOM	2363		TIP S		59.892	15.434	11.467	1.00 31.39	S
									1.00 34.07	
	ATOM	2364		TIP S		31.040	12.361	35.470		S
	ATOM	2365			139	33.489	14.292	-0.598	1.00 40.68	S
	MOTA	2366	OH2	TIP S	140	46.918	8.748	11.662	1.00 29.23	S
40	ATOM	2367	OH2 !	TIP S	141	46.297	-7.287	-9.196	1.00 42.20	S
	ATOM	2368	ОН2 '			58.193	6.715	-4.685	1.00 35.48	S
	ATOM	2369			143	44.598	4.435	12.503	1.00 27.68	S
	ATOM	2370	OH2			27.003	5.999	12.450	1.00 36.30	S
	MOTA	2371	OH2	TIP S	145	43.676	32.852	35.735	1.00 35.70	S
45	ATOM	2372	OH2 !	TIP S	146	35.783	18.628	36.452	1.00 34.62	S
	ATOM	2373	ОН2 '	סדיד ס	147	25.402	4.058	20.638	1.00 45.03	S
	ATOM	2374	OH2			45.839	35.853	33.724	1.00 35.47	S
	MOTA	2375	OH2	rip S	149	22.176	18.976	16.752	1.00 31.87	S
	MOTA	2376	OH2	TIP S	150	43.986	33.179	10.162	1.00 37.70	S
50	ATOM	2377	OH2 '	TIP S	151	50.653	20.347	42.428	1.00 35.80	S
	ATOM	2378			152	47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379			153	44.693		-14.175	1.00 29.90	S
	ATOM	2380	OH2			26.560	36.851	31.684	1.00 49.29	S
	ATOM	2381	OH2	TIP S	156	46.867	8.019	-12.951	1.00 29.21	S
55	ATOM	2382			157	30.432	28.741	12.438	1.00 37.76	S
	ATOM	2383			158	41.004	20.553	6.423	1.00 39.53	S
	ATOM	2384			159	49.258	20.069	29.294	1.00 33.97	S
	ATOM	2385			160	48.082	28.459	16.489	1.00 33.10	S
	ATOM	2386	OH2 !	TIP S	161	47.448	18.625	27.683	1.00 34.87	S

	ATOM	2387	OH2	TIP	S	162	19.687	20.632	23.411	1.00	35.01	S
	ATOM	2388	OH2	TIP	S	163	32.402	-1.266	22.443	1.00	37.26	S
	ATOM	2389		TIP			39.475	33.468			35.34	S
	MOTA	2390	OH2	TIP	S	165	44.277	18.950	5.162	1.00	45.14	S
5	ATOM	2391	OH2	TIP	S	166	34.797	30.523	10.736	1.00	47.55	S
	ATOM	2392		TIP		167	46.541		-14.949		26.54	S
	ATOM	2393	OH2	TIP	S	168	36.333	16.371	1.539	1.00	38.68	S
	MOTA	2394	OH2	TIP	S	169	46.761	38.936	27.403	1.00	34.66	S
	ATOM	2395	OH2	TIP	S	170	24.163	13.264	11.375	1.00	41.23	S
10	ATOM	2396		TIP			48.459	15.018			38.11	S
10												
	ATOM	2397	OH2	TIP	S	172	34.261	23.193	40.004	1.00	48.96	S
	ATOM	2398	OH2	TIP	S	173	45.924	-0.026	13.224	1.00	39.55	S
	ATOM	2399	OH2	TIP	S	175	41.384	37.389	32.543	1 00	40.74	S
		2400		TIP		177	49.394	35.312			44.33	S
	ATOM											
15	MOTA	2401	OH2	TIP	S	178	29.066	29.942	34.359	1.00	41.46	S
	ATOM	2402	OH2	TIP	S	180	49.354	19.467	7.273	1.00	34.56	S
	ATOM	2403	OH2	TIP	S	181	25.298	17.029	31.863	1 00	47.74	S
	MOTA	2404		TIP			37.071	25.027			43.87	S
	ATOM	2405	OH2	TIP	S	183	22.581	7.487	18.691	1.00	41.75	S
20	ATOM	2406	OH2	TIP	S	184	32.269	7.011	-1.891	1.00	48.84	S
	ATOM	2407					48.234	0.494			48.16	S
	MOTA	2408		TIP		187	20.008	14.658			45.27	S
	ATOM	2409	OH2	TIP	S	188	49.341	22.698	42.272	1.00	42.20	S
	ATOM	2410	OH2	TIP	S	190	61.292	18.260	-8.097	1.00	45.21	S
25	ATOM	2411	OH2	TIP	S	191	28.152	10.606		1 00	40.38	S
23												
	ATOM	2412	OH2			192	25.626				34.27	S
	ATOM	2413	OH2	TIP	S	193	59.876	11.603	1.216	1.00	46.54	S
	ATOM	2414	OH2	TIP	S	194	57.592	21.183	-10.646	1.00	45.82	S
	ATOM	2415	OH2	TIP			31.509	36.649			38.73	S
20												
30	ATOM	2416	OH2				50.270	-1.543			42.66	S
	ATOM	2417	OH2	TIP	S	198	24.467	8.729	13.088	1.00	42.78	S
	ATOM	2418	OH2	TIP	S	199	38.098	8.699	25.759	1.00	32.80	S
	ATOM	2419	OH2	TIP			57.831		-13.255		45.31	S
	ATOM	2420	OH2	TIP			23.888	22.328			37.12	S
35	ATOM	2421	OH2	TIP	S	202	47.691	26.068	37.666	1.00	37.92	S
	ATOM	2422	OH2	TIP	S	203	38.653	7.070	29.307	1.00	50.54	S
	ATOM	2423	ОН2	TIP	S	206	44.424	27.583	2.092	1 00	53.50	S
	MOTA	2424	OH2	TIP			22.258	2.296			47.38	S
	ATOM	2425	OH2	TIP	S	214	19.843	17.943	23.303	1.00	30.36	S
40	ATOM	2426	OH2	TIP	S	216	27.647	11.344	24.681	1.00	31.32	S
	ATOM	2427	OH2	TIP	S	217	37.953	7.817	-9.284	1 00	45.97	S
							33.845	34.040				
	ATOM	2428	OH2								38.11	S
	ATOM	2429		TIP			58.484	15.269			38.26	S
	MOTA	2430	OH2	TIP	S	220	48.526	40.920	26.583	1.00	35.23	S
45	ATOM	2431	OH2	TIP	S	222	52.094	21.184	38.122	1.00	29.86	S
				TIP								S
	MOTA	2432					36.889				37.63	
	ATOM	2433	OH2	TIP	S	224	47.642	-1.401	-10.684	1.00	34.89	S
	MOTA	2434	OH2	TIP	S	226	47.284	2.916	19.133	1.00	34.10	S
	ATOM	2435	OH2	TIP	S	227	42.468		-15.039	1.00	37.98	S
50				TIP							41.57	
50	ATOM	2436					19.169					S
	MOTA	2437	OH2	TIP	S	231	57.592	12.689	14.880	1.00	50.22	S
	ATOM	2438	OH2	TIP	S	232	27.102	9.176	5.655	1.00	40.57	S
	ATOM	2439		TIP			58.618		-11.925		50.71	S
	ATOM	2440		TIP			22.822	25.342			34.93	S
55	MOTA	2441	OH2	TIP	S	236	24.831	32.218	28.901	1.00	37.69	S
	MOTA	2442	OH2	TIP	S	237	20.045	10.774	16.992	1.00	39.57	S
	ATOM	2443		TIP			58.019				41.42	S
	ATOM	2444		TIP			19.490				34.55	S
	MOTA	2445	OH2	TIP	S	240	61.187	26.377	7.346	1.00	39.68	S

	MOTA	2446	OH2 TIP	s 241	33.680	38.342	19.389	1.00 48.93	S
	ATOM	2447	OH2 TIE	S 242	51.539	31.612	10.881	1.00 55.65	S
	ATOM	2448	OH2 TIE		25.872	14.431	30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP		37.332	5.849	9.544	1.00 43.81	S
5	MOTA	2450	OH2 TIP	S 250	39.087	-1.293	-9.655	1.00 42.96	S
	ATOM	2451	OH2 TIE	s 258	23.938	30.000	30.010	1.00 38.89	S
	ATOM	2452	OH2 TIE		24.949	29.749	32.578	1.00 40.17	S
							1.918	1.00 48.36	S
	ATOM	2453			32.111	17.986			
	ATOM	2454	OH2 TIP		21.404	12.876	25.603	1.00 57.17	S
10	MOTA	2455	OH2 TIP	S 269	35.425	36.767	12.550	1.00 30.70	S
	MOTA	2456	OH2 TIE	s 270	52.438	25.529	30.131	1.00 44.85	S
	ATOM	2457	OH2 TIE	s 271	53.299	20.156	36.003	1.00 37.15	S
	ATOM	2458	OH2 TIE		50.914	6.919	23.723	1.00 43.29	S
		2459	OH2 TIE		31.578	30.795		1.00 50.15	S
1.5	ATOM						11.014		
15	ATOM	2460	OH2 TIE		26.341	7.243	22.447	1.00 39.40	S
	ATOM	2461	OH2 TIE	S 276	60.392	18.195	10.235	1.00 37.91	S
	ATOM	2462	OH2 TIE	s 277	47.355	-9.081	-10.821	1.00 48.18	S
	ATOM	2463	OH2 TIE	s 279	41.304	6.175	-16.647	1.00 38.12	S
	ATOM	2464	OH2 TIE		33.299	21.620	37.881	1.00 46.29	S
20									
20	ATOM	2465	OH2 TIP		56.469	26.112	-8.575	1.00 43.71	S
	MOTA	2466		S 287	48.382	26.573	7.246	1.00 41.43	S
	MOTA	2467	OH2 TIE	S 288	56.240	7.245	-11.331	1.00 41.79	S
	ATOM	2468	OH2 TIE	s 290	49.060	14.978	28.166	1.00 37.03	S
	ATOM	2469	OH2 TIE	S 291	37.095	44.270	26.442	1.00 45.08	S
25	ATOM	2470	OH2 TIE		47.814		-13.299	1.00 48.60	S
23									
	ATOM	2471		S 297	58.081	2.784	-7.841	1.00 41.89	S
	MOTA	2472	OH2 TIE	S 298	36.447	45.321	18.644	1.00 54.91	S
	MOTA	2473	OH2 TIE	S 299	49.029	23.328	1.767	1.00 30.55	S
	ATOM	2474	OH2 TIE	s 301	24.375	13.771	8.634	1.00 48.47	S
30	ATOM	2475	OH2 TIE		47.904	36.798	28.653	1.00 35.76	S
50	ATOM	2476	OH2 TIE		51.156	40.821	27.172	1.00 43.59	S
	ATOM	2477	OH2 TIP		32.943	28.917	35.227	1.00 42.60	S
	MOTA	2478	OH2 TIP	s 307	58.462	28.373	6.251	1.00 46.15	S
	MOTA	2479	OH2 TIE	s 308	41.964	30.940	36.712	1.00 48.26	S
35	ATOM	2480	OH2 TIE	s 313	51.176	-1.922	-3.336	1.00 50.61	S
	ATOM	2481	OH2 TIE	s1001	21.319	36.868	23.805	1.00 36.97	S
	ATOM	2482		s1002	48.880	32.620	27.617	1.00 44.40	S
	ATOM	2483		S1003	61.880	19.473	11.767	1.00 45.49	S
	ATOM	2484		s1004	52.770	21.424	26.815	1.00 24.43	S
40	MOTA	2485	OH2 TIP	s1005	35.373	29.094	36.197	1.00 35.97	S
	MOTA	2486	OH2 TIE	s1006	40.815	-6.636	4.389	1.00 43.15	S
	ATOM	2487	OH2 TIE	s1007	44.953	1.286	11.272	1.00 49.45	S
	ATOM	2488	OH2 TIE		21.004	16.168	27.009	1.00 48.51	S
	ATOM	2489	OH2 TIE		47.094	41.786	9.243	1.00 50.10	S
4.5									
45	ATOM	2490	OH2 TIE		32.479	2.978	14.158	1.00 49.47	S
	MOTA	2491	012 GLC	G 1	48.557	11.372	-12.279	1.00 40.72	G
	ATOM	2492	C11 GLC	G 1	48.836	12.133	-11.097	1.00 38.05	G
	ATOM	2493	C13 GLC	G 1	49.266	13.554	-11.476	1.00 38.09	G
	ATOM	2494	014 GLC		49.559		-10.292	1.00 33.99	G
50			C15 GLC				-12.257		
30	ATOM	2495			48.150			1.00 37.32	G
	ATOM	2496	016 GLC		48.574		-12.604	1.00 36.74	G
	MOTA	2497	012 GLC	G 2	40.114	-6.634	-6.562	1.00 33.52	G
	MOTA	2498	C11 GLC	G 2	38.967	-6.592	-7.404	1.00 31.05	G
	ATOM	2499	C13 GLC	G 2	37.712	-6.417	-6.552	1.00 31.56	G
55	ATOM	2500	014 GLC		36.554	-6.406	-7.389	1.00 30.70	G
22									
	ATOM	2501	C15 GLC		37.792	-5.109	-5.761	1.00 30.03	G
	ATOM	2502	016 GLC		36.609	-4.961	-4.975	1.00 29.66	G
	ATOM	2503	012 GLC		44.030		-13.470	1.00 37.90	G
	ATOM	2504	C11 GLC	G 3	43.950	9.648	-13.690	1.00 38.47	G

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	ATOM	2505		GLC		3		2.747		-14.579		39.52	G
	MOTA	2506		GLC	G	3		1.551		-13.942		39.39	G
	MOTA	2507	C15	GLC	G	3	4	2.878	9.280	-15.934	1.00	41.43	G
	ATOM	2508	016	GLC	G	3	4	1.736	9 613	-16.731	1 00	40.78	G
-													
5	MOTA	2509		GLC		5		0.556	1.005	2.289		45.25	G
	ATOM	2510	C11	GLC	G	5	4	0.966	2.332	1.960	1.00	40.56	G
	MOTA	2511	C13	GLC	G	5	4	0.187	3.327	2.814	1.00	40.36	G
	ATOM	2512	014	GLC	G	5	3	8.791	3.169	2.572	1 00	40.71	G
				GLC		5			4.751				
1.0	ATOM	2513						0.619		2.464		40.04	G
10	ATOM	2514	016	GLC	G	5	3	9.885	5.681	3.256		36.89	G
	MOTA	2515	012	GLC	G	6	3	6.951	22.702	40.046	1.00	63.04	G
	ATOM	2516	C11	GLC	G	6	3	7.592	21.583	39.422	1.00	62.46	G
	ATOM	2517		GLC		6		8.104	21.978	38.030		61.14	G
	MOTA	2518		GLC		6	3	9.034	23.054	38.168		61.72	G
15	MOTA	2519	C15	GLC	G	6	3	6.948	22.429	37.126	1.00	60.51	G
	ATOM	2520	016	GLC	G	6	3	5.992	21.372	36.960	1.00	58.61	G
	ATOM	2521	012	GLC	G	7	3	7.316	0.281	14.299	1 00	73.45	G
						7							
	ATOM	2522		GLC				7.655	-0.758	15.222		72.78	G
	ATOM	2523	C13	GLC	G	7	3	6.592	-1.856	15.157	1.00	72.98	G
20	ATOM	2524	014	GLC	G	7	3	5.320	-1.299	15.498	1.00	73.88	G
	ATOM	2525	C15	GLC	G	7	3	6.924	-2.989	16.134	1.00	73.66	G
	ATOM	2526		GLC		7		6.972	-2.493	17.478		75.38	G
	ATOM	2527		GLC		8		1.921	21.898	5.908		62.51	G
	MOTA	2528	C11	GLC	G	8	5	2.447	20.871	5.063	1.00	63.42	G
25	ATOM	2529	C13	GLC	G	8	5	1.476	20.597	3.908	1.00	64.28	G
	ATOM	2530	014	GLC	G	8	5	1.297	21.794	3.150	1.00	66.28	G
	ATOM	2531		GLC		8		0.121	20.137	4.448		64.49	G
	MOTA	2532		GLC		8		9.233	19.886	3.357		64.01	G
	MOTA	2533	012	GLC	G	10	3	6.044	37.499	29.523	1.00	56.89	G
30	ATOM	2534	C11	GLC	G	10	3	5.164	36.645	30.259	1.00	56.97	G
	ATOM	2535	C13	GLC	G	10	3	3.849	36.489	29.494	1.00	56.11	G
	ATOM	2536		GLC		10		3.248	37.772	29.308		56.44	G
	MOTA	2537		GLC		10		2.900	35.580	30.277		55.84	G
	MOTA	2538	016	GLC	G	10	3	1.674	35.442	29.557	1.00	55.39	G
35	ATOM	2539	03G	ATP	N	1	4	6.280	25.658	5.170	1.00	51.49	N
	ATOM	2540	PG	ATP	N	1	4	6.464	25.053	3.691	1.00	52.22	N
	ATOM	2541		ATP	N	1		7.406	23.911	3.763		51.41	N
	ATOM	2542			Ν	1		6.794	26.182	2.784		52.07	N
	MOTA	2543	03В	ATP	N	1	4	4.976	24.513	3.344	1.00	51.01	N
40	ATOM	2544	PB	ATP	N	1	4	4.560	22.969	3.605	1.00	50.20	N
	ATOM	2545	01B	ATP	Ν	1	4	3.083	22.898	3.669		49.41	N
	ATOM	2546		ATP		1		5.345	22.474	4.766		50.34	N
						_							
	MOTA	2547	03A	ATP		1		5.070	22.231	2.255		47.77	N
	MOTA	2548	PA	ATP	N	1	4	5.075	20.613	2.121	1.00	42.84	N
45	ATOM	2549	01A	ATP	N	1	4	5.547	20.291	0.754	1.00	43.81	N
	ATOM	2550	02 A	ATP	M	1	4	5.807	20.035	3.270	1.00	45.03	N
	ATOM	2551		ATP		1		3.516	20.223	2.245		41.73	N
	ATOM	2552		ATP		1		2.528	20.925	1.489		37.57	N
	ATOM	2553	C4*	ATP	Ν	1	4	1.127	20.379	1.776	1.00	39.45	N
50	ATOM	2554	04*	ATP	Ν	1	4	0.907	19.024	1.279	1.00	37.72	N
	ATOM	2555		ATP		1		0.777	20.321	3.251	1 00	38.48	N
						1						40.42	
	ATOM	2556		ATP				0.360	21.615	3.697			N
	ATOM	2557		ATP		1		9.608	19.374	3.270		37.58	N
	MOTA	2558	02*	ATP	N	1	3	8.410	20.076	2.924	1.00	35.98	N
55	ATOM	2559	C1*	ATP	Ν	1	3	9.939	18.346	2.173	1.00	35.55	N
	ATOM	2560	N9	ATP		1		0.628	17.156	2.747		31.76	N
	ATOM	2561	C8	ATP		1		1.864	17.126	3.274		30.49	N
	ATOM	2562	Ν7	ATP		1		2.143	15.877	3.667		29.75	N
	ATOM	2563	С5	ATP	N	1	4	1.088	15.118	3.390	1.00	27.49	N

	ATOM	2564	C4	ATP	N	1	40.125	15.925	2.810	1.00 30.02	N
	ATOM	2565	N3	ATP	N	1	38.937	15.389	2.431	1.00 27.11	. N
	ATOM	2566	C2	ATP	N	1	38.679	14.085	2.615	1.00 25.62	N
	ATOM	2567	N1	ATP	N	1	39.597	13.283	3.175	1.00 21.76	N
5	ATOM	2568	С6	ATP	N	1	40.800	13.768	3.571	1.00 23.90	N
	ATOM	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00 21.94	N
	ATOM	2570	S	SO4	I	1	58.680	8.493	-0.639	1.00 56.05	I
	ATOM	2571	01	SO4	I	1	57.956	7.875	0.483	1.00 58.83	I
	ATOM	2572	02	SO4	I	1	57.886	9.607	-1.188	1.00 57.04	I
10	ATOM	2573	03	SO4	I	1	58.906	7.478	-1.683	1.00 57.47	I
	ATOM	2574	04	SO4	Ι	1	59.976	9.008	-0.156	1.00 57.51	I
	ATOM	2575	S	SO4	I	2	39.339	4.855	7.057	1.00 84.24	I
	ATOM	2576	01	SO4	I	2	39.390	6.175	7.711	1.00 85.02	I
	ATOM	2577	02	SO4	I	2	40.101	4.897	5.797	1.00 84.75	I
15	ATOM	2578	03	SO4	I	2	37.936	4.506	6.766	1.00 84.94	I
	ATOM	2579	04	SO4	I	2	39.931	3.842	7.954	1.00 84.44	I
	ATOM	2580	S	SO4	I	3	38.987	-2.256	3.310	1.00 58.58	I
	ATOM	2581	01	SO4	I	3	37.734	-1.675	3.827	1.00 59.11	I
	ATOM	2582	02	SO4	I	3	39.460	-1.454	2.172	1.00 59.91	I
20	ATOM	2583	03	SO4	I	3	38.743	-3.640	2.866	1.00 60.97	I
	ATOM	2584	04	SO4	I	3	40.014	-2.260	4.369	1.00 59.58	I
	ATOM	2585	S	SO4	Ι	4	34.397	5.289	30.981	1.00 64.34	I
	ATOM	2586	01	SO4	I	4	33.627	6.528	30.742	1.00 60.43	I
	ATOM	2587	02	SO4	Ι	4	34.337	4.427	29.782	1.00 60.11	
25	ATOM	2588	03	SO4	I	4	33.816	4.572	32.133	1.00 64.39	I
	ATOM	2589	04	SO4	I	4	35.806	5.626	31.277	1.00 63.55	I
	ATOM	2590	S	SO4	I	5	55.074	-6.984	-3.711	1.00 75.40	
	ATOM	2591	01	SO4	I	5	54.657	-7.518	-2.399	1.00 74.66	
	ATOM	2592	02	SO4	I	5	54.209	-5.845	-4.065	1.00 74.96	I
30	ATOM	2593	03	SO4	I	5	54.950	-8.034	-4.742	1.00 74.22	
	ATOM	2594	04	SO4	I	5	56.477	-6.532	-3.633	1.00 75.15	
	ATOM	2595	02	PO4	Ρ	100	57.362	24.998	13.149	1.00 66.76	P
	ATOM	2596	03	PO4	Ρ	100	59.399	26.166	13.761	1.00 66.89	
	ATOM	2597	04	PO4	Ρ	100	57.761	25.606	15.462	1.00 67.43	
35	ATOM	2598	01	PO4	Ρ	100	57.264	27.325	13.818	1.00 65.91	
	ATOM	2599	P	PO4	Ρ	100	57.947	26.025	14.048	1.00 66.69	P
	END										

Example 5: PDK1 fragments

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We produced constructs for expression of different forms of PDK1 in bacteria. The constructs were either in TRC vectors, pET-15b vector and pGEX expression vector to enable the expression of GST fused N-terminally to PDK1. PDK1 expressed from pGEX 51-556 (ie residues 51 to 556 of PDK1) was found to be highly degraded.

PDK1 protein was also expressed with N-terminal His tags from vector TRC comprising PDK1 sequences 51-556, 51-404 and 1-360, or pET15b 51-404 and tested for expression levels and activity. The expression was generally low, around 0.2 mg/L culture. The specific activity was lower than the His-tagged 51-556 protein purified from baculovirus cells. In the case of PDK1 51-404 expressed from pET-15b construct the level of expression turned out to be very variable. This was probably due to instability of the plasmid since we produced evidence that after a growth of 0.2 units of absorbance, (as measured in a spectrophotometer at 600 nm wavelength) the cells growing faster in the culture were actually not harbouring the plasmid with ampiciline resistance. The instability of the plasmid can be due to toxicity produced by basal expression of PDK1. Although production in bacteria was the theoretical best expression system to avoid heterogeneity due to the different extent of phosphorylation of the different phosphorylation sites in hPDK1, it was found that the protein was either degraded, expressed to low levels, had 5 times less specific activity, or was possibly toxic.

The His-tagged purified PDK1 51-556 protein obtained from baculovirus expression system was homogeneous as depicted by the appearance of one band after by SDS-PAGE analysis of a sample.

Nevertheless, the analysis after isoelectric focussing revealed a large smear of protein covering several units of pH. This analysis suggested that the protein was not homogeneous in terms of its isoelectric point, possibly due to the number of phosphorylation sites which were not homogeneously phosphorylated. This protein did not crystallise.

We purified to homogeneity a truncated His-Myc tagged PDK1 (51-404) which lacks the N-terminal 50 residues and the C-terminal 152 residues which include the PH domain. This protein, produced by a baculovirus expression system, had similar characteristics to the full length wild type PDK1 in terms of its activity towards the peptide substrate T308tide, its activation by the peptide PIFtide, and the binding to PIFtide (as analysed by BiaCore). The purified protein was screened for crystallisation conditions using Hampton Research kits (144 different conditions). Crystallisation conditions were screened with two concentrations of PDK1, in the presence or absence of PIFtide, Staurosporine, at 20°C and in the presence of PIFtide at 4°C. No protein crystals were observed after 6 months, suggesting that this construct was not suitable for forming crystals although all other characteristics were similar to wild type protein.

The His-Myc PDK1 51-404 purified protein was also subjected to protease treatments in order to obtain a protease-insensitive molecule for increasing the chances of obtaining a shorter, stable variant of PDK1. Different protease treatments were tested. Treatment with Glu-C produced a polypeptide of approximately 38 KDa which was stable. This PDK1 protein was active and lacked the His-tag and part of the Myc-tag, and possibly part of the C-terminal residues. This protein was also set up for crystallography screenings. Some crystals were obtained using this preparation after 4 months, but they were not followed up.

A protein kinase corresponding to residues PDk1 51-387 was also produced, in an identical vector to that used to produce the protein PDK1 51-359. Interestingly, this protein was similar to wild type and PDK1 51-404, but had extreme problems for concentration using conventional methods. The protein could not be concentrated further than 2.5 mg/ml, and no crystals were obtained using this construct.

The PDK1 protein that finally crystallised is lacking the first 50 aminoacids and was constructed to end at position 359. This protein was stable in the absence of the PH domain and aminoacids that in hPDK1 link the catalytic domain with the PH domain. The construct PDK1 51-359 was also short enough that no other described phosphorylation sites besides activation loop phosphorylation site 241 were present.

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Example 6: Structural basis for UCN-01 specificity and PDK1 inhibition

The staurosporine derivative UCN-01 (7- hydroxyl staurosporine) has been reported to be a potent inhibitor for PDK1 and is currently in clinical trials for the treatment of cancer. Here we report the crystal structures of staurosporine and UCN-01 in complex with the kinase domain of PDK1. We show that although staurosporine and UCN-01 interact with the PDK1 active site in an overall similar manner, the UCN-01 7-hydroxylgroup, which is not present on staurosporine, generates direct and water-mediated hydrogen bonds with active site residues. Inhibition data from UCN-01 tested against a panel of 29 different kinases show a different pattern of inhibition compared to staurosporine. We discuss how these differences in inhibition could be attributed to specific interactions with the additional 7-hydroxyl-group as well as by the size of the 7-hydroxyl-binding pocket. This information could lead to opportunities for structure-based optimisation of PDK1 inhibitors.

Insulin and growth factor signalling is mediated by the activation of a lipid kinase, phosphatidylinositol-3-kinase (PI3K), which produces the second phosphatidylinositol(3,4,5)trisphosphate messenger molecule (PtdIns(3,4,5)P) [1]. Upon generation of PtdIns(3,4,5)P, 3-Phosphoinositide Dependent protein Kinase-1 (PDK1) and protein kinase B (PKB, also known as Akt) are co-localised at the plasma membrane through interaction of their Pleckstrin Homology (PH) domains with PtdIns(3,4,5)P [2, 3]. PDK1 activates PKB by phosphorylation of its T-loop (Thr308 in PKB) [4, 5]. PDK1 also activates other protein kinases related to PKB, including isoforms of p70 ribosomal S6 kinase (S6K) [6], serum and glucocorticoid responsive kinases (SGK) [7] and p90 ribosomal S6 kinase (Rsk) [8]. These kinases lack PH domains and do not bind PtdIns(3,4,5)P3, and are thought to be activated by a different mechanism, in which the substrates require a priming phosphorylation in a conserved hydrophobic motif (HM) at their Cterminus (reviewed in [9]). This phosphorylation creates a docking motif that specifically interacts with a pocket on the N-terminal lobe of the PDK1 kinase domain (termed PDK1 interacting fragment (PIF) pocket) [10, 11] bringing PDK1 together with its substrate and enabling PDK1 to phosphorylate these kinases in their T-loop, thereby activating them. A significant number of human cancers possess elevated PtdIns(3,4,5)Plevels due to mutations in a number of genes that regulate the production and degradation of this 3-phosphoinositide. One of the most frequently found mutations occurs in the PtdIns(3,4,5)P 3-phosphatase (PTEN) resulting in constitutive activation of PKB and S6K, which are thought to be major contributors to the proliferation and the survival of such tumour cells [12]. Thus, inhibitors of PDK1 have the potential to act as anti-cancer agents as they would be expected to suppress activation of S6K and PKB and inhibit cell growth and induce apoptosis of cancer cells that possess elevated levels of PtdIns(3,4,5)P.

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PDK1 consists of an N-terminal kinase domain and a C-terminal PHdomain [13]. The structure of the PDK1 kinase domain has been solved (see the preceding Examples and [11]) and leads to a definition of the residues lining the ATP binding site and an understanding of the PDK1 activation mechanism. The PIFbinding pocket could be identified, together with a specific pocket for the phosphorylated Ser/Thr residue on the HM of substrate kinases. Staurosporine, a natural product ATP-competitive inhibitor, inhibits many kinases in the low nM range [14], and therefore displays a high cytotoxicity [15]. UCN-01 (7-hydroxyl staurosporine) is a derivative with an additional hydroxyl group on the lactam ring (Fig. 1). It was originally described as a PKC-selective inhibitor isolated from Streptomyces sp. cultures [16], although further studies showed it to be more non-specific [14, 17]. UCN-01 potently inhibits the growth and induces apoptosis of many cancer cells and these effects are thought to be unrelated to PKC inhibition [18, 19]. Due to its anti-tumour activity in vivo and in vitro, UCN-01 is currently undergoing clinical trials with positive effects being reported in the phase 1 studies (reviewed in [19]). Recent reports suggested the cell cycle checkpoint kinase Chk1 [20] and PDK1 [21] may be key targets of UCN-01 in inhibiting the growth of cancer cells, as both kinases are inhibited by UCN-01 in the low nM range.

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Here we report the structures of the PDK1 kinase domain in complex with staurosporine and UCN-01, demonstrating the presence of a pocket that accommodates the 7-hydroxyl group of UCN- 01. Specificity tests against a panel of 29 kinases shows that although both staurosporine and UCN-01 are relatively non-specific inhibitors, the fingerprint analysis of UCN-01 inhibition with a panel of protein kinases is significantly different from that of staurosporine. We also perform analysis of residues predicted to line the UCN-01 hydroxyl pocket on a number or protein kinases, and propose a

general model that could account for the different sensitivity of protein kinases for staurosporine and UCN-01.

Methods

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5 Expression, purification and crystallisation

Human PDK1 (residues 51-359) was expressed using a baculovirus mediated infection of the SF21 insect cell line and purified as described in the preceding examples and [11] with the following differences: After elution of the His-tagged protein from the Ni-NTA-agarose beads with 200 mM imidazole, the protein was dialysed against 250 mM NaCl, 25 mM Tris pH 7.5, 1 mM DTT for 3 hours at 4°C. Proteolysis with GST-tagged PreScission protease was performed overnight at 4 °C.

For crystals of the PDK1-UCN-01 complex, 100 µl of PDK1 at a concentration of 6.6 mg/ml was mixed with 30 µl UCN-01 (5.3 mM in 50 % ethanol) and incubated on ice for 2 hours. The protein was crystallized using sitting drop vapour diffusion. 1.25 µl of protein solution was mixed with 0.25 µl cobaltous chloride hexahydrate (0.1 M) and 1 µl mother liquor, consisting of 2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 8.5. Hexagonal, rod-shaped crystals grew at 20 °C and reached a maximum size of 0.05 x 0.05 x 0.3 mm after 7 days. After soaking for 3 seconds in a cryoprotection solution (2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 25 % glycerol) crystals were frozen in a stream of cold nitrogen.

PDK1 in complex with staurosporine was crystallized using the hanging drop technique. Drops consisted of 1μ1 PDK1 at 7.6 mg/ml, 1 μl mother liquor (2.1 M ammonium sulphate, 0.1 M Tris- HCl pH 7.2) and 0.25 μl staurosporine (10 mM in DMSO). Hexagonal shaped crystals suitable for

data collection appeared after 6 weeks at 20 C. Crystals were soaked in 1.7 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 15% glycerol and frozen in a stream of cold nitrogen.

5 Data collection, structure solution and refinement

Data on the PDK1-staurosporine and PDK1-UCN-01 complexes were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH4. The temperature of the crystals was maintained at 100 K using a nitrogen cryostream. Data were processed using the HKL package [22] with final statistics shown in Table 3. The structures were solved by rigid body refinement with CNS [23] using the previously determined PDK1 structure (See previous Examples, PDB code 1H1W) [11] as a starting model which resulted in an initial R-factor of 0.306 (R $_{\!\mathit{free}} =$ 0.284) for PDK1-staurosporine and 0.299 (R $_{\!\mathit{free}} =$ 0.311) for PDK1-UCN-01. Model building with O [24] and iterative refinement in CNS, including solvent molecules and the T-loop phosphorylation site, resulted in final R-factors as shown in Table 3. The ATP binding site showed well-defined density in the unbiased $|F_o|-|F_c|$, ϕ_{calc} maps for all atoms of staurosporine and UCN-01, including the 7-hydroxyl group (Fig. 8). CNS topologies and coordinates for the inhibitors were generated with PRODRG [25]. No electron density could be observed for residues 51-72 (N-terminus), residues 231-239 (T-loop) and residue 359 (C-terminus) in the PDK1-UCN-01 complex. Residues 51-71 (N-terminus) and 233-238 (Tloop) were disordered in the PDK1-staurosporine complex.

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Determination of inhibition and specificity

Protein kinase assays: PDK1 was assayed for 10 min at 30 °C in a 50 μl assay mixture in 50 mM Tris pH 7.5, 0.1 mM EGTA, 0.1% 2-

mercaptoethanol, containing 100 μM PDK1tide substrate peptide (KTFCGTPEYLAPEVRREPRILSEEEQEMFRDFDYIADWC) (SEQ ID NO:112), 10 mM magnesium acetate, 100 μM [γ-³²P]ATP (200 cpm/pmole) as described previously [10]. Other protein kinases employed in Table 5, were assayed as described previously [17, 26].

Results & Discussion

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Structures of the staurosporine and UCN-01 complexes

PDK1 (residues 51-359) was co-crystallized with staurosporine and UCN-01, and synchrotron diffraction data on a thin hexagonal needle were collected to 2.3 Å and 2.5 Å resolution, respectively.

In the unbiased $|F_o|$ - $|F_c|$, ϕ_{calc} maps well defined (>3.0 σ) density could be observed in the ATP binding site of the kinase, covering all staurosporine/UCN-01 atoms including the 7-hydroxyl group (Fig. 8). After initial rounds of protein model building and inclusion of water molecules, the inhibitor molecules were built and refined with full occupancy to average B-factor of 18.5 Å² (staurosporine) and 17.3 Å²(UCN-01). Further refinement resulted in a final PDK1-staurosporine model with R= 0.218 (R_{free} = 0.255) and a final PDK1-UCN-01 model with R = 0.184 (R_{free} = 0.257), both with good stereochemistry (Table 3).

The staurosporine molecule is located in the ATP-binding site (which lies between the N-terminal and C-terminal lobes of kinases [27, 28]), at the same position described for the inhibitor in complex with the closely related (38 % sequence identity) protein kinase A (PKA, [29], PDB code 1STC) (Fig. 8). Hydrophobic residues on both sides of the ATP binding cleft sandwich the heterocyclic moiety of staurosporine, namely Leu88, Val96, Ala109, Leu98 (small lobe) and Thr222, Leu212 of the larger lobe (Fig. 1).

Similar to the PKA-staurosporine complex, the lactam group mimics the interactions of the adenine base in ATP with the protein backbone, where 2 conserved hydrogen bonds are formed between the lactam-nitrogen N6 in staurosporine (nomenclature according to [30]) and the backbone-oxygen of Ser160, and the lactam-oxygen at the C5 position and the backbone-nitrogen of Ala162 (Table 4). An additional hydrogen bond is mimicked in the staurosporine sugar-moiety, where the methyl-amino group contacts oxygen O 2 of Glu166, similar to the hydrogen bond with the ribose in the PDK1-ATP complex [11], and also the backbone carbonyl of Glu209 (Table 4).

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The UCN-01 molecule occupies the same position in the ATP binding site as staurosporine (maximum atomic shift = 0.35 Å) (Fig. 9). The same hydrophobic interactions are made to the heterocyclic moiety in the PDK1staurosporine complex. Hydrogen bonding interactions to the heterocycle and the sugar moiety are also conserved, with similar geometry (Table 4). However, the 7-hydroxyl group of UCN-01 forms several novel hydrogen bonds (Fig. 9, Table 4). It hydrogen bonds directly to Oy 1 of Thr 222 (Fig. 9, Table 4). In addition, an ordered water molecule (B-factor = 24.0 Å^2) is found in a position where it contacts the 7-hydroxyl (distance = 3.0 Å, Table 4) and the oxygen O ϵ 1 of Gln220 (distance = 2.5 Å) the side chain of which is shifted towards the ligand (1.5 Å for C δ , rotation of 82° around χ_1) compared to the PDK1-STO complex. However, the water molecule is buried in a predominantly hydrophobic pocket, lined by Val143, Leu212 and Cy 2 of Thr222 (Fig. 9). Val143 also changes its position compared to the PDK1-staurosporine complex (Fig. 9), moving further towards the back of the pocket (shift of 0.7 °A for the Cα carbon, and a rotation of 100° around χ_1) and displaces an ordered water molecule present in the PDK1staurosporine complex (Fig. 9), and also observed in other kinasestaurosporine complexes [31, 30]. These changes result in more space to

accommodate the bulky 7-hydroxyl group on UCN-01 as indicated by a 6 °A³ increase in ligand volume (calculated with VOIDOO [32]).

Comparison with Chk1-UCN-01

High resolution data for the Chk1 kinase bound to staurosporine and UCN-01 is available (PDB code 1NVQ [30]). In Chk1, Ser147, the equivalent of Thr222 in PDK1, also hydrogen bonds the UCN-01 7-OH directly. In addition, a water mediated network of hydrogen bonds to UCN-01 is observed. However, in Chk1 the water molecule that hydrogen bonds UCN-01 occupies a different position (shifted 5.2 Å compared to the PDK1-UCN-01 complex). Chk1 appears to have a more extended hydrophilic cavity, as there are 2 additional buried water molecules present also in the Chk1-staurosporine complex. The corresponding residue to Gln220 in PDK1 is a Lys (Lys145) in Chk1, which does not interact with the ligand but points away from it.

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UCN-01 inhibition and specificity

PDK1 inhibition by UCN-01 and staurosporine was measured using kinase assays with P^{32} -labelled ATP. PDK1 is inhibited by UCN-01 with an IC₅₀ value of 5 nM, and by staurosporine with an IC₅₀ of 6.5 nM. As a measure for overall specificity of UCN-01 and staurosporine, the effect of these inhibitors was tested against a panel of 29 protein kinases as described previously [17, 26]. The results are shown in Table 5 as percentage of control activity. These data further confirm that UCN-01 and staurosporine are aspecific inhibitors. UCN-01 at 1 μ M concentration reduces the activity of nine kinases in the panel to less than 10%, and of ten others to below 60% of control activity. Staurosporine at 1 μ M will inhibit twelve kinases to less than 10% control activity, and another ten to below 60%. Interestingly, however, several of the protein kinases were differentially inhibited by

staurosporine and UCN-01 (Table 5). In an attempt to understand these differences the panel of kinases was divided in four distinct classes: (a) similar inhibition, (b) stronger inhibition by staurosporine than by UCN-01, (c) stronger inhibition by UCN-01 than by staurosporine, and (d) no inhibition (Table 5). As the additional 7-hydroxyl group is the only difference in the ligand molecules (Fig. 8), and staurosporine and UCN-01 occupy the same position with similar interactions in the binding site (Fig. 9), the residues contacting the extra hydroxyl group were identified for PDK1 and extracted from a sequence alignment of all protein kinases used in the panel (Table 5). A structure-based sequence alignment of known kinase structures was obtained from [33], which was used to validate the sequence-based sequence alignment (Table 5). The nature of the side chains lining the hydroxyl-pocket could provide a partial explanation for the relative difference between UCN-01 and staurosporine inhibition. Two trends can be observed. For the kinases that are inhibited by UCN-01, there appears to be a preference for a side chain capable of hydrogen bonding the 7-hydroxyl in the hydroxyl-pocket. This is in agreement with the presence of a Thr/Ser residue that hydrogen bonds the 7-hydroxyl in the structures of PDK1 (Thr222) and Chk1 (Ser147) bound to UCN-01. Seven out of ten kinases that are hit equally by staurosporine and UCN-01 (group (a)) appear to have a potential hydrogen bonding residue (Table 5). The kinases that are more potently inhibited by UCN-01 than by staurosporine (group (c)) contain a Thr at the Thr222 equivalent position (Table 5). Five out of nine kinases that are inhibited more potently by staurosporine than by UCN-01 (group (b)) lack a potential hydrogen binding partner in the 7-hydroxylpocket (Table 5).

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A second trend which appears to determine specificity is the size of the residues lining the hydroxyl-pocket. If the predicted total volume of the residues (calculated with the BL- set of side chain volumes [34]) at the

positions indicated in Table 5 is set against the activity in the presence of UCN-01, a correlation coefficient of 0.6 is obtained. This suggests that despite inaccuracies in this approach, such as the absence of structural information on precise side chain conformation and water molecules, a weak correlation between predicted hydroxyl pocket volume and UCN-01 inhibition exists. For instance, PKA contains a possible hydrogen bonding partner for UCN-01 (Thr183), but Met134 in the centre of the hydroxyl pocket may leave no space for the extra hydroxyl group (Table 5). A similar arrangement of residues can be observed for MAPKAP-K2 (Table 5). This size dependency may also play a role for the protein kinases neither hit by staurosporine nor UCN-01. The sequence alignment shows that the Val143 and Thr222 equivalent residues are replaced by bulkier Leu or Ile residues in several of the Mitogen Activated Protein Kinase families (Table 5). To investigate the effect of these bulkier side chains on the hydroxyl pocket, we, starting from the PDK1 crystal structure, replaced residues Val143 with Ile and Thr222 with Leu in standard side chain rotamers (in O [24]), which indeed resulted in van der Waals clashes with C7 of staurosporine (shortest distances: 2.8 Å for Leu222, 3.5 Å for Ile143), and may therefore explain the lack of susceptibility towards UCN-01 in the Mitogen Activated Protein Kinase families. CDK2 is inhibited by both staurosporine and UCN-01 similarly, however this kinase lacks a hydrogen bonding partner for the 7-hydroxyl and contains a bulky Phe (Phe80) at the Leu159 equivalent position. In a superposition of CDK2-staurosporine structure [31] with PDK1-UCN-01 (RMSD = 1.3Å on C α atoms) staurosporine is seen to be shifted by 1.2 Å out of the potential hydroxyl pocket due to presence of the bulky Phe80. Interaction of the 7-hydroxyl on UCN-01 was described to be water mediated in CDK2 due to the lack of hydrogen bonding residues [35]. This particular example highlights the limitations of the approach described above. Other examples where none of the described effects account for the observed behaviour are AMPK and

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MSK1. Both MSK1 and SGK1 show the same sequence in their hydroxyl-pocket with Thr406/Thr407, respectively, as potential hydrogen bonding partners, but both were placed in different groups. MSK1 activity is abolished by 1 μ M staurosporine, but shows residual activity (11 %) with UCN-01. SGK1 activity is at 25% of control activity with 1 μ M UCN-01, but twice as high with staurosporine.

Conclusions

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UCN-01 was subjected to a specificity analysis against an in-house panel of 29 protein kinases. Contrary to the suggestions of some previous reports, the data show that UCN-01 is not a specific inhibitor as it inhibited more than half of the tested kinases at significant levels. A direct comparison with staurosporine, however, showed a different pattern of inhibition, and was the subject of further analysis. We have reported the crystal structures of PDK1 in complex with the inhibitors staurosporine and UCN-01. Both inhibitors appear to bind to PDK1 in a similar fashion compared to the Chk1-UCN-01 or PKA-staurosporine [29] complex, with additional hydrogen bonding interactions at the UCN-01 7-hydroxyl group. This moiety is hydrogen bonded directly to Thr222 and indirectly via an ordered water molecule to Gln220. A different water-mediated hydrogen bonding network is also observed in other UCN-01 complexes known to date [35, 30], and might serve as a starting point for further structure-based optimisation. The residues around the 7-hydroxyl group ("hydroxylpocket") were aligned with known kinase structures and kinases sequences. It is apparent that spatial effects in the identified pocket play a key role in determining UCN-01 inhibition, as does the presence of hydrogen bonding partners for the additional hydroxyl group.

Table 3

Details of data collection & structure refinement. Values between brackets are for the highest resolution shell. Crystals were cryo-cooled to 100 K. All measured data were included in structure refinement.

Dataset	Staurosporine	UCN-01
Space group	P3 ₂ 21	P3 ₂ 21
Cell dimensions (Å)	a=124.17	a=123.39
	b=124.17	b=123.39
	c=47.31	c=47.12
Resolution range (Å)	25-2.30 (2.38-2.30)	25-2.50 (2.59-2.50)
# Observed reflections	31730 (3091)	68515 (6290)
# Unique reflections	18018 (1794)	14395 (1430)
Redundancy	1.8 (1.7)	4.8 (4.4)
Ι/σΙ	7.5 (1.8)	4.5 (2.6)
Completeness (%)	95.8 (95.8)	100.0 (99.9)
R _{merge}	0.096 (0.505)	0.167 (0.688)
R _{cryst} , R _{free}	0.218, 0.255	0.189, 0.257
RMSD from ideal		
geometry		
Bonds (Å)	0.007	0.009
Angles (°)	1.7	1.8
B-factor RMSD (Å)	1.5	1.4
(bonded, main chain)		
 protein (Å)	31.5	27.3
 inhibitor (Å)	18.5	17.4

Table 4
Hydrogen bonding between inhibitors and PDK1. Hydrogen bonds between PDK1 and UCN-01 / staurosporine (STO) were calculated with WHAT IF [36] using the HB2 algorithm [37]. This algorithm gives a 0 (no hydrogen bond) to 1 (optimal hydrogen bond) score to reflect hydrogen bond geometry (HB2 column). Donor-acceptor distances are also listed (D-A).

Inhibitor	Protein/H	UCN-01	UCN-01	STO D-A	STO	Comment
	₂ O	D-A (Å)	HB2	(Å)	HB2	
O5	N-	2.8	0.76	3.0	0.81	Conserved
	Ala162					
N6	O-Ser162	2.9	0.80	3.1	0.67	Conserved
N4'	O-	3.2	0.68	3.1	0.39	Conserved
	Glu209					
N4'	Οε2-	2.6	0.63	2.5	0.45	Conserved
	Glu166					
O7	Ογ1-	3.0	0.56			7-hydroxyl
	Thr222					
O7	H ₂ O	3.0	0.89			Water
						mediated to
						(Οε1-
						Gln220)

Table 5
Comparison of inhibition by UCN-01 vs. staurosporine and hydroxyl pocket-lining residues.

The indicated protein kinases were assayed at 0.1 mM ATP as described previously [17, 26], in the absence or presence of 1µM staurosporine (STO) or UCN-01. Results are presented as percentage of kinase activity compared to that in control incubations. The activity results displayed in the two columns are an average of a triplicate determination. Abbreviations not

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defined in main text: ROCKII, Rho-dependent protein kinase-II; AMPK, AMP-activated protein kinase; MKK1, MAP-kinase kinase-1; PRAK, p38regulated/activated protein kinase; PHK, phosphorylase kinase; CK2, Casein kinase-2; CHK1, cell cycle checkpoint kinase-1; DYRK, dual specificity tyrosine phosphorylated and regulated kinase; CSK, C-terminal Src kinase. Residues lining the hydroxyl pocket are shown in the last five columns, as derived from a multiple sequence alignment with T-Coffee [38].

UCN-Kinase **STO** 01

Both STO and UCN-01 inhibit

PDK1	5 ± 1	0 ± 1	Met13	Val14	Leu15	Gln22	Thr22
PDKI	3 ± 1	0 ± 1	4	3	9	0	2
CHK1 (1NVQ [<u>30</u>])	3 ± 1	1 ± 0	Ile	Val	Leu	Lys14 5	Ser147
ΡΚCα	8 ± 2	1 ± 0	Leu	Thr	Met	Lys	Ala
AMPK	0 ± 0	1 ± 1	Leu	Ile	Met	Lys	Ala
PHOS.KINASE (1PHK [39])	2 ± 3	1 ± 2	Leu	Ile	Phe	Lys	Thr
Lck (1QPJ [40])	0 ± 0	3 ± 1	Met	Val	Thr	Lys	Ala
CDK2/cyclin A (1AQ1 [31])	12 ±	8 ± 0	Leu	Val	Phe80	Lys	Ala
PKBΔPH (1O6K [<u>41</u>])	8 ± 2	9 ± 1	Leu	Thr	Met	Lys	Thr
ROCK-II	9 ± 5	13 ± 2	Met	Val	Met	Lys	Ala
S6K1	24 ± 8	21 ± 4	Leu	Val	Leu	Lys	Thr
GSK3β (1I09 [<u>42]</u>)	29 ± 6	25 ± 5	Met	Val	Leu	Lys	Cys
STO inhibits stronger than	ì						

UCN-01

MSK1 $1 \pm 0 \ 11 \pm 0 \ \text{Leu}$ Val Leu Val Thr40

					6
DYRK1α	2 ± 2 15 ± 2 Leu	Met	Phe	Lys	Val
PKA (1STC [<u>29]</u>)	4 ± 1 27 ± 2 Leu	Val	Met13	Gln	Thr18
MKK1	5 ± 8 53 ± 1 Leu	Val	Met	Lys	Cys
MAPKAP-K2	$23 \pm 1 \ 60 \pm 1 \ His$	Val	Met	Lys	Thr
CSK (1BYG [<u>43</u>])	$25 \pm 8 \ 58 \pm 3 \ \text{Met}$	Val	Thr	Lys	Ser
SAPK3/p38γ (1CM8 [<u>44</u>])	$37 \pm 0 \ 94 \pm 8 \ \text{Leu}$	Ile	Met	Lys	Leu
SAPK4/p38δ	$40 \pm 5\ 100 \pm 7 \text{Leu}$	Ile	Met	Lys	Leu
PRAK	$48 \pm 1 \ 89 \pm 4 \ His$	Val	Met	Lys	Cys
UCN-01 inhibits stronge	r				
than STO					
MAPKAP-K1a	18 ± 1 ± 1 Leu	Val	Leu	Lys	Thr34
SGK1	51 ± 4 22 ± 4 Leu	Val	Leu	Val	Thr40 7
Neither UCN-01 nor STC)				
inhibits					
MAPK2/ERK2 (1ERK [45])	100 ± 4 $107 \pm 5 \text{ Leu}$	Ile	Gln	Lys	Cys
JNKSAPK1c	$91 \pm 3 \ 112 \pm 6 \text{Met}$	Ile	Met	Lys	Leu
SAPK2α/p38 (1P38 [<u>46</u>])	$76 \pm 4\ 107 \pm 5 \text{Leu}$	Ile	Thr	Lys	Leu
SAPK2β/p38β2	84 ± 106 ± 4 Leu	Ile	Thr	Arg	Leu
CK2 (1F0Q [<u>47</u>])	95 ± 4 102 ± Leu	Val	Phe	Arg	Ile
CK1 (1CKI [<u>48</u>])	95 ± 96 ± 0 Tyr	Pro	Met	Tyr	Ile

NEK6 $\frac{109 \pm}{2} 80 \pm 7 \text{ Leu} \quad \text{Ile} \quad \text{Leu} \quad \text{Lys} \quad \text{Gly}$

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Example 7: Co-ordinates for PDK1 fragment co-crystallised with

Staurosporine

REMARK coordinates from restrained individual B-factor refinement REMARK refinement resolution: 25.0 - 2.30 A REMARK starting r= 0.2196 free r= 0.2545 REMARK final r = 0.2182 free r = 0.2553REMARK B rmsd for bonded mainchain atoms= 1.536 target= 1.5 REMARK B rmsd for bonded sidechain atoms= 2.154 target= 2.0 REMARK B rmsd for angle mainchain atoms= 2.576 target= 2.0 REMARK B rmsd for angle sidechain atoms= 3.220 target= 2.5 REMARK rweight= 0.1000 (with wa= 2.58634) REMARK target= mlf steps= 30 REMARK sg= P3(2)21 a= 124.172 b= 124.172 c= 47.314 alpha= 90 beta= 90 gamma= 120 REMARK parameter file 1 : /ddl/david/projects/MY CNS/prot.par REMARK parameter file 2 : /ddl/david/projects/MY_CNS/sto.par REMARK parameter file 3 : CNS_TOPPAR:water_rep.param REMARK parameter file 4 : CNS_TOPPAR:ion.param REMARK parameter file 5 : /ddl/david/projects/MY_CNS/glycerol.par REMARK molecular structure file: ../generate/alternate.mtf REMARK input coordinates: ../minimize/minimize.pdb REMARK reflection file= ../../1/hkl/cns.hkl REMARK ncs= none REMARK B-correction resolution: 6.0 - 2.30 REMARK initial B-factor correction applied to fobs : REMARK B11= -4.525 B22= -4.525 B33= 9.049 REMARK B12= -1.949 B13= 0.000 B23= 0.000 REMARK B-factor correction applied to coordinate array B: -0.209 REMARK bulk solvent: density level= 0.340909 e/A^3, B-factor= 36.8807 30 A^2 REMARK reflections with |Fobs|/sigma F < 0.0 rejected REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range: 18858 (100.0 %) REMARK number of unobserved reflections (no entry or |F|=0): 846 (4.5 %) REMARK number of reflections rejected: 0 (0.0 %) REMARK total number of reflections used: 18012 (95.5 %) REMARK number of reflections in working set: 17259 (REMARK number of reflections in test set: 753 (4.0 %) CRYST1 124.172 124.172 47.314 90.00 90.00 120.00 P 32 2 1 REMARK FILENAME="bindividual.pdb" REMARK DATE:30-Jan-2003 19:44:02 created by user: david REMARK VERSION: 1.0 64.267 -7.345 13.422 1.00 74.69 A ATOM 1 CB PRO A 72 63.278 -8.432 13.027 1.00 74.97 A ATOM 2 CG PRO A 72 3 C PRO A 72 65.866 -6.007 12.013 1.00 73.72 A ATOM MOTA 4 O PRO A 72 66.500 -6.002 10.955 1.00 73.74 A 5 N PRO A 72 MOTA 64.256 -7.651 11.034 1.00 74.67 A 6 CD PRO A 72 63.762 -8.901 11.640 1.00 75.33 A MOTA 7 CA PRO A 72 64.474 -6.635 12... 66.329 -5.474 13.141 1.00 72.17 A 67.635 -4.829 13.221 1.00 70.49 A 55 64.474 -6.639 12.090 1.00 74.30 A ATOM 8 N GLNA 73 ATOM

9 CA GLN A 73

ATOM

	ATOM	10	СВ	GLN A	73	67.570	-3.424	12.611	1.00	69.71 A
	ATOM	11	CG	GLN A	73	66.670	-2.458	13.363	1.00	68.72 A
								12.795		69.01 A
	ATOM	12	CD	GLN A	73	66.722	-1.054			
	ATOM	13	OE1	GLN A	73	67.785	-0.435	12.735	0.00	68.92 A
5	ATOM	14	NE2	GLN A	73	65.571	-0.541	12.376	0.00	68.92 A
	ATOM	15	С	GLN A	73	68.057	-4.728	14.683	1.00	
	ATOM	16	0	GLN A	73	67.267	-5.015	15.585	1.00	69.69 A
	ATOM	17	N	PRO A	74	69.313	-4.321	14.940	1 00	68.34 A
	ATOM	18	CD	PRO A	74	70.411	-4.026	13.999	1.00	
10	ATOM	19	CA	PRO A	74	69.769	-4.204	16.330	1.00	67.15 A
	ATOM	20	СВ	PRO A	74	71.198	-3.675	16.178	1.00	67.56 A
	ATOM	21	CG	PRO A	74	71.635	-4.254	14.855		67.46 A
	ATOM	22	С	PRO A	74	68.866	-3.240	17.105	1.00	65.27 A
	ATOM	23	0	PRO A	74	68.496	-2.186	16.584	1.00	65.27 A
1.5										
15	ATOM	24	N	ARG A	75	68.506	-3.598	18.337		62.56 A
	ATOM	25	CA	ARG A	75	67.642	-2.730	19.136	1.00	59.53 A
	ATOM	26	СВ	ARG A	75	67.543	-3.228	20.582	1.00	62.40 A
	ATOM	27	CG	ARG A	75	66.120	-3.565	21.023		64.22 A
	ATOM	28	CD	ARG A	75	66.020	-3.746	22.537	1.00	66.65 A
20	ATOM	29	NE	ARG A	75	64.741	-4.332	22.943		68.76 A
20										
	ATOM	30	CZ	ARG A	75	64.390	-4.572	24.204		70.18 A
	ATOM	31	NH1	ARG A	75	65.218	-4.272	25.197	1.00	70.31 A
	ATOM	32	NH2	ARG A	75	63.213	-5.125	24.477	1.00	71.64 A
	ATOM	33	С	ARG A	75	68.184	-1.306	19.126		55.61 A
25	ATOM	34	0	ARG A	75	69.386	-1.082	18.961	1.00	55.58 A
	ATOM	35	N	LYS A	76	67.294	-0.341	19.295	1.00	50.06 A
								19.297		45.50 A
	ATOM	36	CA	LYS A	76	67.704	1.050			
	ATOM	37	СВ	LYS A	76	66.498	1.941	19.594	1.00	45.42 A
	ATOM	38	CG	LYS A	76	66.404	3.192	18.735	1.00	45.70 A
30	ATOM	39	CD	LYS A	76	66.329	2.829	17.257		44.53 A
30										
	ATOM	40	CE	LYS A	76	66.030	4.045	16.396		44.45 A
	ATOM	41	NZ	LYS A	76	66.091	3.733	14.939	1.00	43.30 A
	ATOM	42	С	LYS A	76	68.783	1.251	20.359	1.00	42.73 A
	ATOM	43	0	LYS A	76	68.715	0.681	21.447		42.46 A
35	ATOM	44	N	LYS A	77	69.793	2.046	20.038	1.00	39.63 A
	ATOM	45	CA	LYS A	77	70.851	2.309	20.995	1.00	36.33 A
	ATOM	46	СВ	LYS A	77	72.139	2.670	20.267		36.33 A
	ATOM	47	CG	LYS A	77	72.655	1.570	19.353		36.55 A
	ATOM	48	CD	LYS A	77	74.005	1.945	18.785	1.00	35.61 A
40	ATOM	49	CE	LYS A	77	74.491	0.932	17.766	1 00	38.34 A
10										
	ATOM	50	NZ	LYS A	77	74.706	-0.419	18.354		38.65 A
	ATOM	51	С	LYS A	77	70.413	3.459	21.889	1.00	35.52 A
	ATOM	52	0	LYS A	77	69.475	4.190	21.557	1.00	32.62 A
					78					
	ATOM	53	N	ARG A		71.097	3.608	23.020		34.95 A
45	ATOM	54	CA	ARG A	78	70.801	4.654	23.991	1.00	33.79 A
	ATOM	55	СВ	ARG A	78	69.917	4.094	25.114	1.00	35.78 A
	ATOM	56	CG	ARG A	78	70.211	2.652	25.483		38.18 A
	ATOM	57	$^{\rm CD}$	ARG A	78	69.036	2.040	26.239	1.00	38.81 A
	ATOM	58	NE	ARG A	78	68.995	0.578	26.160	0.00	38.43 A
50										
50	ATOM	59	CZ	ARG A	78	69.889	-0.232	26.719		38.44 A
	ATOM	60	NH1	ARG A	78	70.906	0.274	27.401	0.00	38.37 A
	ATOM	61	NH2	ARG A	78	69.760	-1.549	26.610	0.00	38.37 A
				ARG A	78		5.230			
	ATOM	62	С			72.099		24.544		31.96 A
	ATOM	63	0	ARG A	78	73.133	4.576	24.515	1.00	32.75 A
55	ATOM	64	N	PRO A	79	72.060	6.470	25.055	1.00	30.51 A
		65			79					
	ATOM		CD	PRO A		70.844	7.272	25.274		27.35 A
	ATOM	66	CA	PRO A	79	73.236	7.150	25.611		29.82 A
	ATOM	67	СВ	PRO A	79	72.626	8.326	26.365	1.00	28.52 A
	ATOM	68	CG	PRO A	79	71.418	8.628	25.559		29.89 A
	111 011	00	00	INO A	, ,	, 1 • 110	0.020	20.000	1.00	20.00 A

					_						
	ATOM	69	С	PRO A		79	74.129	6.298	26.510		30.92 A
	ATOM	70	0	PRO A	4	79	75.356	6.357	26.412		33.32 A
	ATOM	71	N	GLU A	3 F	80	73.516	5.510	27.383	1.00	29.85 A
	ATOM	72	CA	GLU A	3 A	80	74.273	4.677	28.300	1.00	31.98 A
5	ATOM	73	СВ	GLU A	3 A	80	73.327	3.941	29.242		34.31 A
_	ATOM	74	CG	GLU A		80	72.697	2.710	28.622		41.92 A
	ATOM	75	CD	GLU A		80	71.205	2.626	28.872		44.52 A
	ATOM	76		GLU A		80	70.461	3.466	28.317		46.38 A
	ATOM	77		GLU A		80	70.780	1.721	29.625		46.03 A
10	ATOM	78	С	GLU A	3 E	80	75.157	3.663	27.578		30.62 A
	ATOM	79	0	GLU A	<i>P</i>	80	76.101	3.144	28.170	1.00	30.21 A
	ATOM	80	N	ASP A	3 F	81	74.859	3.378	26.312	1.00	28.14 A
	ATOM	81	CA	ASP A	<i>A</i>	81	75.659	2.417	25.548	1.00	27.32 A
	ATOM	82	СВ	ASP A	3 A	81	74.938	1.990	24.253	1.00	27.75 A
15	ATOM	83	CG	ASP A		81	73.612	1.275	24.512		30.45 A
15	ATOM	84		ASP A		81	73.495	0.549	25.525		30.76 A
		85		ASP A		81	72.686	1.424	23.686		30.74 A
	ATOM										
	ATOM	86	С	ASP A		81	77.026	2.990	25.166		26.35 A
	ATOM	87	0	ASP A		81	77.895	2.266	24.680		25.33 A
20	ATOM	88	N	PHE A	<i>F</i>	82	77.217	4.283	25.404		24.95 A
	ATOM	89	CA	PHE A	<i>P</i>	82	78.457	4.948	25.035	1.00	23.57 A
	ATOM	90	CB	PHE A	3 F	82	78.168	6.040	23.991	1.00	23.02 A
	ATOM	91	CG	PHE A	<i>A</i>	82	77.507	5.534	22.742	1.00	23.64 A
	ATOM	92	CD1	PHE A	3 4	82	78.270	5.059	21.680		23.15 A
25	ATOM	93	CD2	PHE A		82	76.123	5.504	22.640		23.41 A
23	ATOM	94	CE1	PHE A		82	77.670	4.559	20.540		23.43 A
		95	CE2	PHE A		82	75.504	5.003	21.498		24.29 A
	ATOM										
	ATOM	96	CZ	PHE A		82	76.283	4.527	20.444		25.15 A
	ATOM	97	С	PHE A		82	79.199	5.609	26.186		24.39 A
30	ATOM	98	0	PHE A	3 F	82	78.647	5.847	27.259		22.78 A
	ATOM	99	N	LYS A	<i>P</i>	83	80.471	5.896	25.932	1.00	22.40 A
	ATOM	100	CA	LYS A	3 F	83	81.294	6.615	26.869	1.00	23.38 A
	ATOM	101	СВ	LYS A	<i>P P P P P P P P P P</i>	83	82.554	5.834	27.250	1.00	24.29 A
	ATOM	102	CG	LYS A	3 A	83	83.453	6.594	28.227	1.00	27.32 A
35	ATOM	103	CD	LYS A		83	84.411	5.675	28.988		31.40 A
00	ATOM	104	CE	LYS A		83	85.321	4.906	28.044		30.06 A
	ATOM	105	NZ	LYS A		83	86.145	5.819	27.207		30.54 A
	ATOM	106	C	LYS A		83	81.656	7.847	26.046		24.47 A
10	ATOM	107	0	LYS A		83	82.518	7.787	25.162		26.09 A
40	ATOM	108	N	PHE A		8 4	80.965	8.951	26.309		21.59 A
	ATOM	109	CA	PHE A		8 4	81.211	10.182	25.583		21.61 A
	ATOM	110	CB	PHE A	<i>P P</i>	8 4	80.073	11.169	25.811	1.00	20.62 A
	ATOM	111	CG	PHE A	3 F	8 4	78.794	10.757	25.159	1.00	20.05 A
	ATOM	112	CD1	PHE A	3 F	84	77.915	9.905	25.805	1.00	18.27 A
45	ATOM	113	CD2	PHE A	<i>A</i>	8 4	78.498	11.176	23.868	1.00	19.96 A
	ATOM	114		PHE A		8 4	76.764	9.473	25.183		19.47 A
	ATOM	115		PHE A		84	77.346	10.748	23.233		21.09 A
	ATOM	116	CZ	PHE A		84		9.894	23.890		20.64 A
				PHE A							
50	ATOM	117	C			84	82.525	10.820	25.966		22.27 A
50	ATOM	118	0	PHE A		8 4	82.900	10.822	27.129		24.09 A
	ATOM	119	N	GLY A		85	83.213	11.371	24.972		22.72 A
	ATOM	120	CA	GLY A	3 F	85	84.496	12.007	25.203	1.00	22.66 A
	ATOM	121	C	GLY A	3 F	85	84.540	13.481	24.839	1.00	22.72 A
	ATOM	122	0	GLY A	3 A	85	83.622	14.228	25.158	1.00	22.51 A
55	ATOM	123	N	LYS A		86	85.608	13.894	24.162		22.49 A
-	ATOM	124	CA	LYS A		86	85.794	15.291	23.784		22.53 A
	ATOM	125	CB	LYS A		86	87.238	15.530	23.333		24.44 A
		126	CB	LYS A		86	87.617	14.804	22.051		26.94 A
	ATOM										
	ATOM	127	CD	LYS A	-1 (86	89.033	15.120	21.594	1.00	29.52 A

	7	100	C.E.	T 37 C 7	0.0	00 166	16 571	01 154	1 00 25 02 7
	ATOM	128	CE	LYS A	86	89.166	16.571	21.154	1.00 35.93 A
	ATOM	129	NZ	LYS A	86	90.505	16.892	20.553	1.00 38.21 A
	MOTA	130	С	LYS A	86	84.857	15.798	22.699	1.00 23.09 A
	ATOM	131	0	LYS A	86	84.295	15.032	21.923	1.00 22.85 A
5	ATOM	132	N	ILE A	87	84.702	17.114	22.664	1.00 22.28 A
	ATOM	133	CA	ILE A	87	83.867	17.780	21.683	1.00 21.22 A
	ATOM	134	СВ	ILE A	87	83.429	19.170	22.204	1.00 22.05 A
		135	CG2	ILE A	87	82.792	19.993	21.076	1.00 22.03 A
	ATOM								
10	ATOM	136	CG1	ILE A	87	82.493	18.998	23.406	1.00 21.65 A
10	ATOM	137	CD1		87	82.159	20.300	24.118	1.00 18.47 A
	MOTA	138	С	ILE A	87	84.707	17.963	20.418	1.00 21.83 A
	ATOM	139	0	ILE A	87	85.782	18.543	20.470	1.00 21.99 A
	ATOM	140	N	LEU A	88	84.226	17.463	19.288	1.00 22.57 A
	ATOM	141	CA	LEU A	88	84.964	17.614	18.039	1.00 22.76 A
15	ATOM	142	СВ	LEU A	88	84.586	16.515	17.044	1.00 20.65 A
13	ATOM	143	CG	LEU A	88	84.899	15.107	17.535	1.00 20.09 A
	ATOM	144		LEU A	88	84.455	14.082	16.502	1.00 17.42 A
	ATOM	145		LEU A	88	86.392	15.004	17.813	1.00 17.76 A
	ATOM	146	С	LEU A	88	84.657	18.964	17.428	1.00 23.53 A
20	ATOM	147	0	LEU A	88	85.512	19.577	16.794	1.00 24.73 A
	ATOM	148	N	GLY A	89	83.430	19.428	17.619	1.00 24.20 A
	ATOM	149	CA	GLY A	89	83.057	20.710	17.062	1.00 28.57 A
	ATOM	150	С	GLY A	89	81.649	21.131	17.431	1.00 32.57 A
	ATOM	151	0	GLY A	89	80.834	20.318	17.882	1.00 32.78 A
25				GLU A			22.412		
25	ATOM	152	N		90	81.363		17.224	1.00 35.17 A
	ATOM	153	CA	GLU A	90	80.063	22.964	17.542	1.00 39.17 A
	ATOM	154	СВ	GLU A	90	80.168	23.853	18.784	1.00 41.47 A
	ATOM	155	CG	GLU A	90	80.112	23.061	20.082	1.00 47.18 A
	ATOM	156	CD	GLU A	90	80.422	23.893	21.313	1.00 50.49 A
30	ATOM	157	OE1	GLU A	90	81.610	24.228	21.526	1.00 51.41 A
	ATOM	158	OE2	GLU A	90	79.476	24.210	22.067	1.00 53.44 A
	ATOM	159	С	GLU A	90	79.436	23.743	16.402	1.00 40.69 A
	ATOM	160	0	GLU A	90	80.110	24.185	15.471	1.00 40.64 A
	ATOM	161	N	GLY A	91	78.121	23.881	16.488	1.00 42.58 A
25									
35	ATOM	162	CA	GLY A	91	77.363	24.618	15.503	1.00 43.40 A
	ATOM	163	С	GLY A	91	76.303	25.335	16.306	1.00 44.83 A
	ATOM	164	0	GLY A	91	76.154	25.083	17.507	1.00 43.64 A
	MOTA	165	N	SER A	92	75.579	26.244	15.669	1.00 47.22 A
	ATOM	166	CA	SER A	92	74.522	26.969	16.366	1.00 48.94 A
40	ATOM	167	СВ	SER A	92	73.961	28.066	15.461	1.00 51.50 A
	ATOM	168	OG	SER A	92	73.663	27.541	14.175	1.00 54.98 A
	ATOM	169	С	SER A	92	73.454	25.928	16.625	1.00 47.87 A
	ATOM	170	0	SER A	92	72.745	25.950	17.635	1.00 47.78 A
		171		PHE A	93	73.392	24.994	15.689	1.00 47.70 A 1.00 46.49 A
15	ATOM		N						
45	ATOM	172	CA	PHE A	93	72.434	23.909	15.697	1.00 46.02 A
	ATOM	173	СВ	PHE A	93	72.297	23.369	14.263	1.00 49.54 A
	MOTA	174	CG	PHE A	93	73.588	23.398	13.459	1.00 50.29 A
	ATOM	175	CD1	PHE A	93	74.301	22.229	13.209	1.00 52.29 A
	MOTA	176	CD2	PHE A	93	74.058	24.593	12.915	1.00 51.94 A
50	ATOM	177		PHE A	93	75.459	22.245	12.424	1.00 52.28 A
	ATOM	178		PHE A	93	75.209	24.622	12.135	1.00 52.58 A
		179	CZ	PHE A	93	75.911	23.443	11.887	1.00 53.99 A
	ATOM								
	ATOM	180	С	PHE A	93	72.700	22.754	16.662	1.00 43.48 A
	ATOM	181	0	PHE A	93	71.772	22.245	17.292	1.00 42.15 A
55	ATOM	182	N	SER A	94	73.955	22.343	16.796	1.00 39.99 A
	ATOM	183	CA	SER A	94	74.245	21.206	17.655	1.00 36.12 A
	ATOM	184	СВ	SER A	94	73.839	19.937	16.921	1.00 38.79 A
	ATOM	185	OG	SER A	94	74.549	19.863	15.695	1.00 40.39 A
	ATOM	186	C	SER A	94	75.697	21.066	18.083	1.00 32.29 A
	7 7 7 01.1	T 0 0)	SHI/ A	J 1	, 5. 031	21.000	10.000	1.00 J2.23 A

	ATOM ATOM	187 188	O N	SER THR		94 95	76.513 76.006	21.962 19.909	17.890 18.655		30.04 Z 28.50 Z	
	ATOM	189	CA	THR		95	77.350	19.614	19.116		26.86	
_	ATOM	190	СВ	THR		95	77.432	19.642	20.652		27.90	
5	MOTA	191		THR		95	76.907	20.882	21.136		32.56	
	ATOM	192	CG2	THR		95	78.874	19.502	21.112		27.77	
	MOTA	193	С	THR	Α	95	77.757	18.225	18.653	1.00	23.70	Α
	MOTA	194	0	THR	Α	95	76.971	17.287	18.724	1.00	24.35 7	Α
	ATOM	195	N	VAL	Α	96	78.991	18.100	18.184	1.00	22.75	Α
10	ATOM	196	CA	VAL	Α	96	79.505	16.813	17.733	1.00	20.60 2	Α
	ATOM	197	СВ	VAL		96	80.139	16.909	16.336		17.79	
	ATOM	198		VAL		96	80.625	15.530	15.898		18.21	
	ATOM	199		VAL		96	79.131	17.447	15.344		13.79	
	ATOM	200	C	VAL		96	80.566	16.351	18.716		21.23	
1.5												
15	ATOM	201	0	VAL		96	81.600	17.006	18.889		22.12	
	ATOM	202	N	VAL		97	80.310	15.220	19.362		22.06	
	MOTA	203	CA	VAL		97	81.244	14.690	20.345		24.07	
	ATOM	204	СВ	VAL	Α	97	80.592	14.680	21.743		24.91	
	MOTA	205	CG1	VAL	Α	97	79.199	14.124	21.649	1.00	28.97	Α
20	MOTA	206	CG2	VAL	Α	97	81.422	13.859	22.715	1.00	27.97	Α
	ATOM	207	С	VAL	Α	97	81.748	13.298	20.002	1.00	23.47	Α
	MOTA	208	0	VAL	Α	97	81.017	12.491	19.436	1.00	26.62 7	Α
	ATOM	209	N	LEU	Α	98	83.007	13.024	20.329	1.00	22.92	Α
	ATOM	210	CA	LEU		98	83.586	11.713	20.063		23.27	
25	ATOM	211	СВ	LEU		98	85.117	11.777	20.110		21.94 7	
	ATOM	212	CG	LEU		98	85.932	10.495	19.854		22.83	
	ATOM	213		LEU		98	85.606	9.924	18.486		23.24	
	ATOM	214	CD1	LEU		98	87.422	10.802	19.945		21.21	
20	ATOM	215	C	LEU		98	83.069	10.782	21.144		23.95	
30	ATOM	216	0	LEU		98	83.143	11.099	22.322		26.02	
	ATOM	217	N	ALA		99	82.523	9.645	20.738		24.41	
	ATOM	218	CA	ALA		99	81.999	8.677	21.686		23.76	
	MOTA	219	СВ	ALA		99	80.485	8.692	21.668		20.64	
	MOTA	220	С	ALA		99	82.502	7.282	21.357		26.42	
35	MOTA	221	0	ALA	Α	99	82.792	6.951	20.195	1.00	26.78	Α
	MOTA	222	N	ARG	Α	100	82.602	6.462	22.394	1.00	26.77	Α
	MOTA	223	CA	ARG	Α	100	83.055	5.094	22.238	1.00	26.80 7	Α
	ATOM	224	СВ	ARG	Α	100	84.362	4.897	23.001	1.00	28.29	Α
	ATOM	225	CG	ARG	Α	100	84.967	3.522	22.853	1.00	33.87	Α
40	ATOM	226	CD	ARG	Α	100	86.281	3.447	23.617	1.00	38.01 7	Α
	ATOM	227	NE	ARG			87.337	4.240	22.983		41.22	
	ATOM	228	CZ	ARG			87.932	3.917	21.837		41.46	
	ATOM	229		ARG			87.580	2.813			41.28	
	ATOM	230		ARG			88.887	4.692	21.339		43.39	
45	ATOM	231	C	ARG			81.970	4.167	22.770		24.32	
73			0								25.42	
	ATOM	232		ARG			81.583	4.251	23.934			
	ATOM	233	N	GLU			81.456	3.308	21.900		22.41	
	ATOM	234		GLU			80.417	2.367	22.281		22.87	
	ATOM	235	СВ	GLU			79.787	1.775	21.025		21.96	
50	MOTA	236	CG	GLU			78.819	0.652	21.292		24.68	
	ATOM	237	CD	GLU			78.203	0.137	20.018	1.00	28.27	A
	MOTA	238	OE1	GLU	Α	101	78.965	-0.113	19.057	1.00	28.96	Α
	MOTA	239	OE2	GLU	Α	101	76.963	-0.022	19.971	1.00	29.77	Α
	ATOM	240	С	GLU	Α	101	81.015	1.261	23.151	1.00	23.59	Α
55	ATOM	241	0	GLU	Α	101	81.945	0.574	22.738		24.80 7	
	ATOM	242	N			102	80.475	1.088			26.09	
	ATOM	243	CA	LEU			80.982	0.083	25.289		28.74	
											·	
	ATOM	244	СВ	LEU	Α	102	80.173	0.110	26.593	1.00	30.16	A

	ATOM	245	CG	LEU A	102	80.347	1.308	27.532	1.00 34.19 A
	ATOM	246	CD1	LEU A	102	81.824	1.692	27.599	1.00 33.27 A
	ATOM	247	CD2			79.527	2.477	27.046	1.00 34.46 A
_	ATOM	248	С	LEU A		81.042	-1.359	24.791	1.00 28.32 A
5	ATOM	249	0	LEU A		82.067	-2.024	24.916	1.00 29.83 A
	ATOM	250	N	ALA A	103	79.948	-1.841	24.226	1.00 27.34 A
	ATOM	251	CA	ALA A	103	79.887	-3.218	23.763	1.00 27.81 A
	ATOM	252	СВ	ALA A		78.466	-3.549	23.367	1.00 27.48 A
	ATOM	253	С	ALA A		80.828	-3.593	22.624	1.00 27.42 A
10	ATOM	254	0	ALA A	103	81.172	-4.765	22.463	1.00 28.68 A
	ATOM	255	N	THR A	104	81.257	-2.612	21.842	1.00 24.97 A
	ATOM	256	CA	THR A	104	82.105	-2.907	20.695	1.00 23.79 A
	ATOM	257	СВ	THR A		81.441	-2.472	19.393	1.00 22.01 A
	ATOM	258		THR A		81.355	-1.041	19.379	1.00 23.91 A
15	ATOM	259	CG2	THR A		80.051	-3.069	19.261	1.00 17.30 A
	ATOM	260	С	THR A	104	83.444	-2.221	20.712	1.00 25.00 A
	ATOM	261	0	THR A	104	84.350	-2.616	19.972	1.00 25.02 A
	ATOM	262	N	SER A		83.551	-1.172	21.525	1.00 24.89 A
• •	ATOM	263	CA	SER A		84.775	-0.394	21.616	1.00 24.55 A
20	ATOM	264	СВ	SER A	105	85.979	-1.334	21.732	1.00 26.36 A
	ATOM	265	OG	SER A	105	87.143	-0.621	22.090	1.00 32.45 A
	ATOM	266	С	SER A	105	84.916	0.514	20.374	1.00 23.38 A
	ATOM	267	0	SER A		85.931	1.175	20.188	1.00 24.92 A
	ATOM	268	N	ARG A		83.888	0.546	19.531	1.00 20.51 A
25	ATOM	269	CA	ARG A		83.906	1.372	18.323	1.00 19.31 A
	MOTA	270	СВ	ARG A	106	82.778	0.947	17.370	1.00 19.05 A
	ATOM	271	CG	ARG A	106	83.099	-0.283	16.520	1.00 15.69 A
	ATOM	272	CD	ARG A	106	81.853	-0.804	15.832	1.00 19.45 A
	ATOM	273	NE	ARG A		82.144	-1.838	14.846	1.00 20.98 A
20									
30	ATOM	274	CZ	ARG A		81.234	-2.673	14.354	1.00 21.77 A
	ATOM	275	NH1	ARG A	106	79.974	-2.599	14.768	1.00 19.65 A
	ATOM	276	NH2	ARG A	106	81.577	-3.560	13.427	1.00 21.43 A
	ATOM	277	С	ARG A	106	83.760	2.858	18.624	1.00 17.84 A
	ATOM	278	0	ARG A		83.022	3.234	19.525	1.00 15.87 A
25									
35	ATOM	279	N	GLU A		84.463	3.691	17.863	1.00 18.23 A
	ATOM	280	CA	GLU A		84.395	5.144	18.039	1.00 22.75 A
	MOTA	281	СВ	GLU A	107	85.773	5.800	17.929	1.00 23.58 A
	ATOM	282	CG	GLU A	107	86.828	5.254	18.859	1.00 32.15 A
	ATOM	283	CD	GLU A	107	88.066	6.131	18.878	1.00 35.04 A
40	ATOM	284		GLU A		88.145	7.019	19.755	1.00 36.99 A
40									
	ATOM	285		GLU A		88.949	5.944	18.007	1.00 37.54 A
	ATOM	286	С	GLU A	107	83.514	5.787	16.982	1.00 21.00 A
	MOTA	287	0	GLU A	107	83.709	5.577	15.787	1.00 21.37 A
	ATOM	288	N	TYR A	108	82.570	6.593	17.437	1.00 19.48 A
45	ATOM	289	CA	TYR A		81.652	7.298	16.559	1.00 18.30 A
15									
	ATOM	290	СВ	TYR A		80.228	6.791	16.754	1.00 17.52 A
	ATOM	291	CG	TYR A		79.993	5.373	16.309	1.00 22.75 A
	ATOM	292	CD1	TYR A	108	79.727	5.075	14.972	1.00 20.94 A
	ATOM	293	CE1	TYR A	108	79.492	3.765	14.571	1.00 23.91 A
50	ATOM	294		TYR A		80.019	4.324	17.231	1.00 19.41 A
20		295				79.788	3.026		1.00 19.33 A
	ATOM			TYR A				16.845	
	ATOM	296	CZ	TYR A		79.527	2.744	15.521	1.00 23.13 A
	MOTA	297	OH	TYR A	108	79.333	1.438	15.143	1.00 23.65 A
	ATOM	298	С	TYR A		81.660	8.777	16.906	1.00 18.00 A
55	ATOM	299	0	TYR A		81.929	9.161	18.046	1.00 18.12 A
22									
	ATOM	300	N	ALA A			9.603	15.912	1.00 17.20 A
	ATOM	301	CA	ALA A		81.274	11.036	16.114	1.00 15.30 A
	ATOM	302	СВ	ALA A	109	81.853	11.784	14.928	1.00 13.44 A
	ATOM	303	С	ALA A	109	79.759	11.205	16.178	1.00 17.20 A

		004	_			1.0.0	E0 0E6	44 040	45 450	4 00	45 00 -
	ATOM	304	0	ALA A			79.056	11.019	15.179		17.23 A
	ATOM	305	N	ILE A	A 1	110	79.250	11.522	17.362		17.40 A
	ATOM	306	CA	ILE A	A 1	110	77.814	11.654	17.542	1.00	17.60 A
	ATOM	307	СВ	ILE A	A 1	110	77.380	10.957	18.842	1.00	16.56 A
5	ATOM	308	CG2	ILE A			75.906	11.236	19.119		14.97 A
5		309	CG1						18.728		
	ATOM			ILE A			77.672	9.453			14.02 A
	ATOM	310	CD1	ILE A			77.197	8.632	19.907		11.93 A
	ATOM	311	С	ILE A	1	110	77.306	13.089	17.548	1.00	19.83 A
	ATOM	312	0	ILE A	A 1	110	77.690	13.892	18.396	1.00	20.84 A
10	ATOM	313	N	LYS A	A 1	111	76.444	13.415	16.597	1.00	18.58 A
	ATOM	314	CA	LYS A			75.902	14.761	16.551		20.88 A
				LYS A			75.455	15.115			21.39 A
	ATOM	315	СВ						15.131		
	ATOM	316	CG	LYS A			75.016	16.558	14.975		24.84 A
	ATOM	317	CD	LYS A	1	111	75.005	16.971	13.516	1.00	27.43 A
15	ATOM	318	CE	LYS A	1	111	74.426	18.359	13.343	1.00	28.44 A
	ATOM	319	NΖ	LYS A	A 1	111	74.619	18.871	11.972	1.00	28.27 A
	ATOM	320	С	LYS A			74.724	14.819	17.507		20.66 A
	ATOM	321	0	LYS A			73.797	14.008	17.410		20.23 A
	ATOM	322	N	ILE A			74.772	15.765	18.441		20.09 A
20	ATOM	323	CA	ILE A	A 1	112	73.704	15.914	19.426	1.00	23.02 A
	ATOM	324	CB	ILE A	A 1	112	74.261	15.882	20.863	1.00	24.20 A
	ATOM	325	CG2	ILE A			73.116	15.765	21.864		21.42 A
	ATOM	326	CG1	ILE A			75.206	14.692	21.023		24.14 A
2.5	ATOM	327	CD1	ILE A			75.893	14.634	22.375		26.83 A
25	ATOM	328	С	ILE A			72.962	17.225	19.221		22.53 A
	ATOM	329	0	ILE A	A 1	112	73.573	18.286	19.132	1.00	21.31 A
	ATOM	330	N	LEU A	A 1	113	71.641	17.138	19.150	1.00	24.04 A
	ATOM	331	CA	LEU A	A 1	113	70.800	18.313	18.940	1.00	25.81 A
	ATOM	332	СВ	LEU A			70.135	18.264	17.555		24.66 A
20		333	CG						16.295		
30	ATOM			LEU A			70.988	18.095			26.73 A
	ATOM	334		LEU A			71.316	16.620	16.093		24.51 A
	ATOM	335	CD2	LEU A			70.234	18.637	15.083	1.00	26.16 A
	ATOM	336	С	LEU A	A 1	113	69.702	18.400	19.994	1.00	27.62 A
	ATOM	337	0	LEU A	A 1	113	69.053	17.398	20.314	1.00	29.70 A
35	ATOM	338	N	GLU A			69.491	19.597	20.530		29.32 A
	ATOM	339	CA	GLU A			68.445	19.806	21.526		31.56 A
	ATOM	340	СВ	GLU A			68.775	21.020	22.391		34.85 A
	ATOM	341	CG	GLU A			67.680	21.357	23.392		42.32 A
	ATOM	342	CD	GLU A	1	114	67.922	22.670	24.108	1.00	45.56 A
40	ATOM	343	OE1	GLU A	A 1	114	68.086	23.700	23.417	1.00	48.01 A
	ATOM	344	OE2	GLU A	A 1	114	67.941	22.673	25.359	1.00	48.10 A
	ATOM	345	С	GLU A	Δ 1	114	67.107	20.036	20.816		31.02 A
	ATOM	346	0	GLU A			66.926	21.049	20.140		30.39 A
4.5	ATOM	347	N	LYS A			66.176	19.099	20.967		30.58 A
45	ATOM	348	CA	LYS A			64.872	19.218	20.321		31.63 A
	ATOM	349	СВ	LYS A	1	115	63.964	18.049	20.734	1.00	28.91 A
	ATOM	350	CG	LYS A	A 1	115	64.287	16.742	20.003	1.00	28.07 A
	ATOM	351	CD	LYS A	A 1	115	63.356	15.580	20.368	1.00	23.95 A
	ATOM	352	CE	LYS A			63.713	14.960	21.707		23.89 A
50											
50	ATOM	353	NΖ	LYS A			62.860	13.782	22.020		24.15 A
	ATOM	354	С	LYS A			64.165	20.551	20.591		33.78 A
	ATOM	355	0	LYS A	A 1	115	63.495	21.100	19.711	1.00	33.61 A
	ATOM	356	N	ARG A	A 1	116	64.325	21.076	21.801	1.00	35.55 A
	ATOM	357	CA	ARG A	A 1	116	63.682	22.332	22.176	1.00	38.66 A
55	ATOM	358	СВ	ARG A			63.932	22.627	23.663		42.20 A
55											
	ATOM	359	CG	ARG A			62.949	23.603	24.302		47.35 A
	ATOM	360	CD	ARG A			63.670	24.685	25.109		52.44 A
	ATOM	361	NE	ARG A			64.526	24.141	26.166		56.30 A
	ATOM	362	CZ	ARG A	1	116	64.142	23.920	27.423	1.00	57.97 A

	7) TI ()M	363	MLI 1	7 D.C	7\	116	62.899	24.199	27.808	1 00	58.89	7\
	ATOM			ARG								
	ATOM	364		ARG			65.006	23.420	28.300		56.55	
	MOTA	365	С	ARG			64.227	23.472	21.323		37.67	
	MOTA	366	0	ARG			63.474	24.246	20.735		36.66	
5	ATOM	367	N	HIS			65.550	23.555	21.259		37.78	
	ATOM	368	CA	HIS	Α	117	66.236	24.590	20.501	1.00	35.88	Α
	MOTA	369	СВ	HIS	Α	117	67.744	24.417	20.676	1.00	35.60	Α
	ATOM	370	CG	HIS	Α	117	68.560	25.532	20.101	1.00	37.06	Α
	ATOM	371	CD2	HIS	Α	117	69.508	25.535	19.134	1.00	38.11	Α
10	ATOM	372	ND1	HIS	Α	117	68.469	26.831	20.550	1.00	37.56	Α
	ATOM	373	CE1	HIS	А	117	69.325	27.587	19.886	1.00	38.35	А
	ATOM	374		HIS			69.969	26.825	19.021		38.67	
	ATOM	375	С	HIS			65.859	24.529	19.024		34.83	
	ATOM	376	0	HIS			65.600	25.554	18.398		35.80	
15	ATOM	377	N	ILE			65.827	23.321	18.474		33.01	
15	ATOM	378	CA	ILE			65.483	23.122	17.071		32.12	
	ATOM	379	CB	ILE			65.575	21.629	16.692		33.37	
		380	CG2	ILE			64.968	21.398	15.312		33.44	
	ATOM											
20	ATOM	381		ILE			67.032	21.168	16.732		33.47	
20	ATOM	382	CD1	ILE			67.195	19.685	16.479		35.01	
	ATOM	383	C	ILE			64.066	23.603	16.760		31.17	
	ATOM	384	0	ILE			63.838	24.295	15.774		29.39	
	ATOM	385	N	ILE			63.117	23.209	17.600		31.17	
2.5	ATOM	386	CA	ILE			61.725	23.590	17.420		31.73	
25	MOTA	387	СВ	ILE			60.841	22.896	18.473		31.45	
	MOTA	388	CG2	ILE			59.471	23.560	18.548		26.98	
	ATOM	389	CG1	ILE			60.735	21.409	18.131		27.55	
	ATOM	390	CD1	ILE			60.092	20.574	19.205		26.52	
	ATOM	391	С	ILE			61.549	25.100	17.519		33.53	
30	MOTA	392	0	ILE			60.879	25.714	16.688		32.81	
	MOTA	393	N	ALA	Α	120	62.165	25.691	18.535	1.00	34.30	Α
	MOTA	394	CA	ALA	Α	120	62.078	27.125	18.749	1.00	34.63	Α
	MOTA	395	СВ	ALA	Α	120	62.811	27.506	20.029	1.00	35.03	Α
	MOTA	396	С	ALA	Α	120	62.657	27.889	17.574	1.00	35.68	Α
35	ATOM	397	0	ALA	Α	120	62.141	28.938	17.195	1.00	36.85	Α
	MOTA	398	N	GLU	Α	121	63.732	27.369	16.995	1.00	35.66	Α
	ATOM	399	CA	GLU	Α	121	64.375	28.041	15.870	1.00	36.43	Α
	ATOM	400	СВ	GLU	Α	121	65.873	27.726	15.864	1.00	40.99	Α
	MOTA	401	CG	GLU	Α	121	66.637	28.166	17.116	1.00	45.01	Α
40	ATOM	402	CD	GLU	Α	121	66.844	29.676	17.205	1.00	48.12	Α
	ATOM	403	OE1	GLU	Α	121	67.670	30.104	18.043	1.00	49.33	Α
	ATOM	404		GLU			66.188	30.433	16.451	1.00	49.20	Α
	ATOM	405	С	GLU			63.780	27.670	14.512		34.98	
	ATOM	406	0	GLU			64.282	28.105	13.480		34.50	
45	ATOM	407	N	ASN			62.716	26.869	14.517		33.68	
	ATOM	408	CA	ASN			62.060	26.434	13.286		32.99	
	ATOM	409	CB	ASN			61.492	27.639	12.530		35.58	
	ATOM	410	CG	ASN			60.424	28.373	13.315		38.88	
	ATOM	411		ASN			60.717	29.154	14.227		38.30	
50	ATOM	412		ASN			59.170	28.116	12.970		38.77	
50	ATOM	413	C	ASN			63.024	25.679	12.370		31.80	
	ATOM	414	0	ASN			63.024	25.957	11.172		30.78	
	ATOM	415	N	LYS			63.754	24.716	12.919		29.93	
55	ATOM	416	CA	LYS			64.717	23.966	12.120		29.87	
55	ATOM	417	CB	LYS			66.100	24.016	12.775		30.75	
	ATOM	418	CG	LYS			66.669	25.406	12.895		33.94	
	ATOM	419	CD	LYS			66.810	26.049	11.527		37.59	
	ATOM	420	CE	LYS			67.354	27.466	11.646		39.07	
	ATOM	421	NZ	LYS	А	123	67.460	28.121	10.310	T.00	41.71	А

	7) III () M	122	C	TVC 7	100	64 227	20 514	11 000	1 00 07 20 7
	ATOM	422	С	LYS A		64.337	22.514	11.880	1.00 27.38 A
	MOTA	423	0	LYS A		65.139	21.745	11.355	1.00 24.93 A
	ATOM	424	N	VAL A	124	63.124	22.132	12.260	1.00 24.22 A
	ATOM	425	CA	VAL A	124	62.716	20.756	12.062	1.00 22.73 A
5	ATOM	426	СВ	VAL A	124	61.235	20.559	12.416	1.00 22.36 A
	ATOM	427	CG1	VAL A		60.794	19.146	12.064	1.00 22.84 A
	ATOM	428	CG2			61.031	20.802	13.905	1.00 20.63 A
		429	C	VAL A		62.981	20.320	10.623	1.00 23.50 A
	ATOM								
10	ATOM	430	0	VAL A		63.633	19.297	10.385	1.00 21.86 A
10	ATOM	431	N	PRO A		62.512	21.109	9.639	1.00 23.91 A
	ATOM	432	CD	PRO A	125	61.806	22.399	9.725	1.00 24.52 A
	ATOM	433	CA	PRO A	125	62.737	20.736	8.239	1.00 24.57 A
	ATOM	434	СВ	PRO A	125	62.147	21.914	7.464	1.00 23.69 A
	ATOM	435	CG	PRO A	125	61.098	22.450	8.400	1.00 25.18 A
15	ATOM	436	С	PRO A		64.217	20.520	7.923	1.00 23.84 A
13	ATOM	437	0	PRO A		64.568	19.618	7.172	1.00 23.01 A
	ATOM	438	N	TYR A		65.073	21.353	8.501	1.00 24.86 A
	ATOM	439	CA	TYR A		66.511	21.259	8.274	1.00 28.10 A
	ATOM	440	СВ	TYR A	126	67.202	22.494	8.859	1.00 32.76 A
20	ATOM	441	CG	TYR A	126	66.802	23.766	8.146	1.00 39.46 A
	ATOM	442	CD1	TYR A	126	67.466	24.179	6.987	1.00 42.04 A
	ATOM	443	CE1	TYR A	126	67.063	25.322	6.292	1.00 43.67 A
	ATOM	444	CD2	TYR A		65.722	24.531	8.597	1.00 42.16 A
	ATOM	445	CE2	TYR A		65.309	25.673	7.909	1.00 43.70 A
25			CZ			65.983	26.062	6.758	1.00 43.70 A 1.00 44.51 A
23	ATOM	446		TYR A					
	ATOM	447	OH	TYR A		65.570	27.183	6.068	1.00 45.30 A
	ATOM	448	С	TYR A		67.115	19.984	8.852	1.00 26.14 A
	ATOM	449	0	TYR A		67.768	19.225	8.141	1.00 26.15 A
	ATOM	450	N	VAL A	127	66.891	19.756	10.141	1.00 24.35 A
30	ATOM	451	CA	VAL A	127	67.396	18.568	10.819	1.00 24.93 A
	ATOM	452	СВ	VAL A	127	66.956	18.568	12.296	1.00 24.24 A
	ATOM	453	CG1	VAL A		67.444	17.316	12.997	1.00 23.36 A
	ATOM	454	CG2	VAL A		67.492	19.809	12.979	1.00 21.11 A
	ATOM	455	C	VAL A		66.894	17.290	10.130	1.00 25.81 A
35									
33	ATOM	456	0	VAL A		67.655	16.351	9.903	1.00 25.79 A
	ATOM	457	N	THR A		65.612	17.273	9.793	1.00 25.57 A
	ATOM	458	CA	THR A		64.996	16.136	9.114	1.00 26.36 A
	ATOM	459	СВ	THR A	128	63.486	16.384	8.908	1.00 25.21 A
	ATOM	460	og1	THR A	128	62.827	16.390	10.181	1.00 29.29 A
40	ATOM	461	CG2	THR A	128	62.883	15.317	8.043	1.00 25.73 A
	ATOM	462	С	THR A	128	65.640	15.898	7.748	1.00 26.97 A
	ATOM	463	0	THR A		65.929	14.760	7.366	1.00 25.68 A
	ATOM	464	N	ARG A		65.854	16.980	7.012	1.00 27.23 A
	ATOM	465	CA	ARG A		66.462	16.897	5.692	1.00 29.37 A
45									
45	ATOM	466	СВ	ARG A		66.484	18.282	5.032	1.00 32.35 A
	ATOM	467	CG	ARG A		66.936	18.280	3.583	1.00 36.81 A
	ATOM	468	CD	ARG A	129	67.208	19.693	3.064	1.00 40.45 A
	ATOM	469	NE	ARG A	129	66.178	20.651	3.459	1.00 44.54 A
	ATOM	470	CZ	ARG A	129	64.874	20.474	3.268	1.00 48.21 A
50	ATOM	471	NH1	ARG A	129	64.431	19.366	2.681	1.00 50.01 A
	ATOM	472		ARG A		64.008	21.403	3.668	1.00 47.79 A
	ATOM	473	С	ARG A		67.884	16.379	5.828	1.00 28.98 A
	ATOM	474	0	ARG A		68.316	15.532	5.054	1.00 28.26 A
	ATOM	475	N	GLU A		68.606	16.895	6.822	1.00 29.28 A
55	ATOM	476	CA	GLU A		69.988	16.490	7.057	1.00 30.58 A
	ATOM	477	СВ	GLU A	130	70.556	17.203	8.287	1.00 34.18 A
	ATOM	478	CG	GLU A	130	72.078	17.220	8.344	1.00 38.81 A
	ATOM	479	CD	GLU A		72.633	17.650	9.702	1.00 41.66 A
	ATOM	480		GLU A		71.946	18.408	10.427	1.00 42.36 A

	MOTA	481	OE2	GLU A	130	73.771	17.236	10.035	1.00	42.31 A
	ATOM	482	С	GLU A	130	70.063	14.984	7.273	1.00	30.12 A
	ATOM	483	0	GLU A	130	70.861	14.298	6.638	1.00	29.62 A
								8.173		
_	MOTA	484	N	ARG A		69.228	14.474			29.21 A
5	MOTA	485	$^{\rm CA}$	ARG A	131	69.215	13.046	8.458	1.00	30.93 A
	ATOM	486	СВ	ARG A	131	68.241	12.724	9.601	1.00	32.88 A
	ATOM	487	CG	ARG A		68.035	11.223	9.795	1.00	36.48 A
							10.885	10.922		41.14 A
	ATOM	488	CD	ARG A		67.069				
	ATOM	489	NE	ARG A	131	66.859	9.440	11.012	1.00	45.98 A
10	ATOM	490	CZ	ARG A	131	66.167	8.833	11.974	1.00	48.77 A
	ATOM	491	NH1	ARG A	131	65.605	9.546	12.946	1 00	48.39 A
	MOTA	492		ARG A		66.045	7.509	11.968		48.16 A
	MOTA	493	С	ARG A	131	68.836	12.226	7.224	1.00	29.97 A
	MOTA	494	0	ARG A	131	69.398	11.157	6.986	1.00	28.24 A
15	ATOM	495	N	ASP A		67.889	12.725	6.437		28.56 A
13										
	MOTA	496	CA	ASP A		67.460	11.996	5.251		29.18 A
	MOTA	497	СВ	ASP A	132	66.160	12.583	4.710	1.00	31.39 A
	MOTA	498	CG	ASP A	132	65.005	12.409	5.682	1.00	38.76 A
	ATOM	499	OD 1	ASP A		64.892	11.319	6.283	1 00	40.09 A
20										
20	MOTA	500		ASP A		64.206	13.355	5.846		44.19 A
	MOTA	501	С	ASP A	132	68.510	11.936	4.150	1.00	27.67 A
	ATOM	502	0	ASP A	132	68.688	10.896	3.522	1.00	27.56 A
	ATOM	503	N	VAL A		69.200	13.044	3.909		26.09 A
	ATOM	504	CA	VAL A		70.232	13.063	2.886		25.09 A
25	MOTA	505	СВ	VAL A	133	70.859	14.459	2.742	1.00	25.26 A
	ATOM	506	CG1	VAL A	133	72.157	14.369	1.961	1.00	24.32 A
	ATOM	507	CG2	VAL A	133	69.890	15.390	2.029	1 00	24.76 A
	MOTA	508	С	VAL A		71.320	12.076	3.266		25.33 A
	MOTA	509	0	VAL A	133	71.742	11.270	2.445	1.00	23.59 A
30	ATOM	510	N	MET A	134	71.764	12.138	4.520	1.00	26.01 A
	ATOM	511	CA	MET A		72.812	11.243	4.995	1 00	27.63 A
	MOTA	512	СВ	MET A		73.210	11.576	6.436		25.11 A
	ATOM	513	CG	MET A		74.056	12.834	6.539	1.00	27.52 A
	ATOM	514	SD	MET A	134	74.875	13.035	8.132	1.00	28.28 A
35	ATOM	515	CE	MET A		73.545	13.741	9.104		28.66 A
55			C	MET A			9.779			28.59 A
	MOTA	516				72.431		4.901		
	ATOM	517	0	MET A	134	73.276	8.938	4.599	1.00	31.12 A
	ATOM	518	N	SER A	135	71.168	9.467	5.165	1.00	29.14 A
	MOTA	519	CA	SER A	135	70.709	8.082	5.090	1.00	31.93 A
40	ATOM	520	СВ	SER A		69.261	7.966	5.558		32.44 A
40										
	MOTA	521	OG	SER A		69.112	8.470	6.868		40.09 A
	MOTA	522	С	SER A	135	70.786	7.557	3.668	1.00	31.36 A
	MOTA	523	0	SER A	135	71.010	6.374	3.454	1.00	32.23 A
	ATOM	524	N	ARG A		70.597	8.448	2.701		31.66 A
15										
45	MOTA	525	CA	ARG A		70.602	8.075	1.293		32.53 A
	MOTA	526	СВ	ARG A	136	69.798	9.095	0.491	1.00	33.51 A
	ATOM	527	CG	ARG A	136	68.361	9.274	0.962	1.00	38.41 A
	ATOM	528	CD	ARG A	136	67.676	10.352	0.137		40.27 A
	MOTA	529	NE	ARG A		67.850	10.090	-1.288		42.75 A
50	ATOM	530	CZ	ARG A	136	67.560	10.953	-2.253		44.58 A
	ATOM	531	NH1	ARG A	136	67.071	12.151	-1.950	1.00	45.74 A
	ATOM	532	NH2	ARG A	136	67.771	10.621	-3.522		43.43 A
	ATOM	533	С	ARG A		71.985	7.946	0.670		32.09 A
	ATOM	534	0	ARG A	136	72.113	7.513	-0.474	1.00	32.48 A
55	ATOM	535	N	LEU A	137	73.019	8.329	1.406	1.00	30.72 A
	ATOM	536	CA	LEU A		74.371	8.253	0.873		30.30 A
	ATOM	537	CB	LEU A		75.167	9.508	1.262		29.84 A
	MOTA	538	CG	LEU A		74.541	10.843	0.831		30.25 A
	MOTA	539	CD1	LEU A	137	75.488	11.963	1.154	1.00	29.16 A

	7.001	F 40	ana			1 2 7	74 020	10 005	0 656	1 00	00 60 7
	ATOM	540		LEU A			74.230	10.835	-0.656		29.68 A
	ATOM	541	С	LEU A			75.083	7.006	1.369		29.52 A
	ATOM	542	0	LEU A	7	137	75.033	6.684	2.553		31.12 A
	ATOM	543	N	ASP A	4	138	75.745	6.310	0.453	1.00	27.02 A
5	ATOM	544	CA	ASP A	4	138	76.467	5.087	0.773	1.00	25.70 A
	ATOM	545	СВ	ASP A			75.556	3.887	0.492	1.00	29.85 A
	ATOM	546	CG	ASP A			76.198	2.567	0.858		33.94 A
	ATOM	547		ASP A			76.815	2.486	1.949		34.64 A
10	ATOM	548		ASP A			76.074	1.610	0.058		35.28 A
10	ATOM	549	С	ASP A			77.699	5.062	-0.127		24.23 A
	ATOM	550	0	ASP A	Ŧ	138	77.765	4.300	-1.091	1.00	24.33 A
	ATOM	551	N	HIS A	1	139	78.672	5.904	0.209	1.00	20.89 A
	ATOM	552	CA	HIS A	Į.	139	79.888	6.069	-0.577	1.00	19.30 A
	ATOM	553	СВ	HIS A			79.681	7.243	-1.553	1.00	17.75 A
15	ATOM	554	CG	HIS A			80.774	7.410	-2.564		17.45 A
13	ATOM	555		HIS A			80.794	7.179	-3.897		16.63 A
		556									
	ATOM			HIS A			82.034	7.862	-2.235		20.01 A
	ATOM	557		HIS A			82.784	7.901	-3.322		16.89 A
	ATOM	558	NE2	HIS A			82.054	7.491	-4.344		16.94 A
20	MOTA	559	С	HIS A	7	139	81.066	6.347	0.352		19.25 A
	ATOM	560	0	HIS A	Ą	139	80.914	6.990	1.388	1.00	21.17 A
	ATOM	561	N	PRO A	Ą	140	82.265	5.881	-0.021	1.00	17.84 A
	ATOM	562	CD	PRO A	4	140	82.575	5.120	-1.243	1.00	16.07 A
	ATOM	563	CA	PRO A			83.467	6.079	0.789		18.04 A
25	ATOM	564	CB	PRO A			84.518	5.240	0.055		18.70 A
23		565		PRO A					-1.365		19.17 A
	ATOM		CG				84.061	5.315			
	ATOM	566	С	PRO A			83.919	7.523	1.014		19.75 A
	ATOM	567	0	PRO A			84.686	7.793	1.930		21.01 A
	ATOM	568	N	PHE A	Į	141	83.460	8.457	0.192	1.00	20.21 A
30	ATOM	569	CA	PHE A	Ŧ	141	83.869	9.837	0.389	1.00	20.05 A
	ATOM	570	СВ	PHE A	1	141	84.149	10.496	-0.964	1.00	20.20 A
	ATOM	571	CG	PHE A	A	141	85.333	9.909	-1.686	1.00	20.95 A
	ATOM	572		PHE A			86.362	9.297	-0.975		21.45 A
	ATOM	573	CD2	PHE A			85.430	9.983	-3.071		20.27 A
35		574		PHE A			87.476	8.765	-1.635		22.05 A
33	ATOM										
	ATOM	575	CE2	PHE A			86.541	9.456	-3.743		20.58 A
	ATOM	576	CZ	PHE A			87.562	8.848	-3.027		20.58 A
	ATOM	577	С	PHE A			82.881	10.679	1.210	1.00	18.71 A
	MOTA	578	0	PHE A	7	141	83.015	11.897	1.300	1.00	19.78 A
40	ATOM	579	N	PHE A	1	142	81.903	10.027	1.823	1.00	18.61 A
	ATOM	580	CA	PHE A	Ā	142	80.915	10.738	2.639	1.00	19.11 A
	ATOM	581	СВ	PHE A	Ā	142	79.543	10.709	1.966	1.00	17.36 A
	ATOM	582	CG	PHE A			79.458	11.565	0.750		19.19 A
	ATOM	583		PHE A			79.258	12.936	0.863		19.44 A
45				PHE A							
43	ATOM	584					79.649	11.016	-0.511		18.39 A
	ATOM	585		PHE A			79.254	13.759	-0.268		20.66 A
	ATOM	586	CE2	PHE A			79.648	11.824	-1.644		20.80 A
	MOTA	587	CZ	PHE A	1	142	79.451	13.203	-1.523		18.95 A
	ATOM	588	С	PHE A	1	142	80.787	10.132	4.023	1.00	18.98 A
50	ATOM	589	0	PHE A	Ā	142	80.735	8.918	4.168	1.00	18.39 A
	ATOM	590	N	VAL A	Ā	143	80.736	10.983	5.041	1.00	20.79 A
	ATOM	591	CA	VAL A			80.578	10.499	6.401		20.94 A
	ATOM	592	CB	VAL A			80.456	11.670	7.404		21.95 A
	ATOM	593		VAL A			80.081	11.145	8.783		21.30 A
55	ATOM	594		VAL A			81.781	12.433	7.473		19.28 A
	ATOM	595	С	VAL A			79.299	9.683	6.396		21.12 A
	ATOM	596	0	VAL A	Ā	143	78.280	10.124	5.895	1.00	23.63 A
	ATOM	597	N	LYS A	4	144	79.367	8.481	6.940	1.00	23.64 A
	ATOM	598	CA	LYS A			78.221	7.582	6.990	1.00	24.47 A

	ATOM	599	СВ	LYS .	Α	144	78.714	6.131	6.869	1.00 25.53 A
	ATOM	600	CG	LYS	Α	144	77.635	5.061	6.997	1.00 32.25 A
	ATOM	601	CD	LYS	Α	144	78.240	3.660	6.870	1.00 36.07 A
	ATOM	602	CE	LYS	Α	144	77.187	2.563	7.033	1.00 38.50 A
5	ATOM	603	NZ	LYS	Α	144	77.791	1.186	7.051	1.00 41.46 A
	ATOM	604	С	LYS	A	144	77.418	7.744	8.275	1.00 22.60 A
	ATOM	605	0	LYS			77.973	8.019		1.00 23.18 A
	ATOM	606	N	LEU			76.104	7.583		1.00 21.59 A
	ATOM	607	CA	LEU			75.224	7.661		1.00 21.42 A
10	ATOM	608	CB	LEU	-1	145	73.918	8.372		0.50 21.42 A
10		609	CG	LEU		145	72.843			0.50 21.21 AC1
	ATOM						73.356			
	ATOM	610	CD1	LEU		145				0.50 19.59 AC1 0.50 21.45 AC1
	ATOM	611		LEU	70	145	71.569	8.994		
1.7	ATOM	612	C	LEU .			74.919	6.215		1.00 21.84 A
15	ATOM	613	0	LEU .			74.283	5.471		1.00 19.24 A
	ATOM	614	N	TYR			75.363	5.816		1.00 19.77 A
	ATOM	615	CA	TYR			75.143	4.444		1.00 19.92 A
	ATOM	616	СВ	TYR			76.326	3.944		1.00 18.05 A
	ATOM	617	CG	TYR	A	146	77.601	3.803		1.00 17.64 A
20	ATOM	618	CD1	TYR	A	146	78.435	4.909		1.00 18.26 A
	ATOM	619	CE1	TYR	A	146	79.638	4.782	10.516	1.00 17.33 A
	ATOM	620	CD2	TYR	Α	146	78.000	2.560	10.910	1.00 15.57 A
	ATOM	621	CE2	TYR	Α	146	79.208	2.419	10.215	1.00 17.53 A
	ATOM	622	CZ	TYR	Α	146	80.022	3.535	10.026	1.00 18.78 A
25	ATOM	623	OH	TYR	Α	146	81.224	3.413	9.369	1.00 19.47 A
	ATOM	624	С	TYR	Α	146	73.884	4.194	12.170	1.00 20.60 A
	ATOM	625	0	TYR	Α	146	73.331	3.100	12.108	1.00 21.73 A
	ATOM	626	N	PHE	Α	147	73.431	5.192	12.921	1.00 20.92 A
	ATOM	627	CA	PHE	Α	147	72.239	5.025	13.745	1.00 22.59 A
30	ATOM	628	СВ	PHE			72.538	4.063		1.00 22.24 A
	ATOM	629	CG	PHE			73.708	4.488		1.00 21.88 A
	ATOM	630	CD1				73.607	5.578		1.00 21.93 A
	ATOM	631	CD2	PHE			74.936	3.843		1.00 21.57 A
	ATOM	632		PHE			74.715	6.025		1.00 25.21 A
35	ATOM	633	CE2	PHE			76.051	4.279		1.00 21.30 A
55	ATOM	634	CZ	PHE			75.942	5.371		1.00 24.23 A
	ATOM	635	C	PHE			71.737	6.343		1.00 24.23 A 1.00 23.77 A
		636	0	PHE			72.448	7.352		1.00 23.77 A 1.00 22.91 A
	ATOM ATOM	637	N	THR			70.501	6.324		1.00 22.91 A 1.00 25.15 A
40										1.00 25.15 A
40	ATOM	638	CA	THR			69.908	7.503		
	ATOM	639	CB	THR			68.953	8.251		1.00 27.00 A
	ATOM	640		THR			67.850	7.400		1.00 27.79 A
	ATOM	641		THR .			69.660	8.661		1.00 26.35 A
4.7	ATOM	642	С	THR			69.080	7.055		1.00 26.23 A
45	ATOM	643	0	THR			68.591	5.930		1.00 26.46 A
	ATOM	644	N	PHE			68.942	7.943		1.00 25.72 A
	ATOM	645	CA	PHE			68.133	7.662		1.00 25.10 A
	ATOM	646	СВ	PHE			68.789	6.593		1.00 23.02 A
	ATOM	647	CG	PHE			70.088	7.011		1.00 22.26 A
50	ATOM	648	CD1	PHE	A	149	70.105	7.794	21.373	1.00 20.98 A
	ATOM	649	CD2	PHE	A	149	71.302	6.587	19.694	1.00 21.51 A
	ATOM	650	CE1	PHE	A	149	71.312	8.151	21.976	1.00 22.36 A
	ATOM	651	CE2	PHE	A	149	72.511	6.939	20.288	1.00 21.06 A
	ATOM	652	CZ	PHE	Α	149	72.519	7.722	21.430	1.00 19.46 A
55	ATOM	653	С	PHE	Α	149	67.931	8.974		1.00 27.05 A
	ATOM	654	0	PHE			68.565	9.974		1.00 27.03 A
	ATOM	655	N	GLN			67.024	8.984		1.00 29.18 A
	ATOM	656	CA	GLN			66.757	10.198		1.00 31.94 A
	ATOM	657	СВ	GLN			65.697	11.035		1.00 32.80 A

	ATOM	658	CG	GLN	Α	150	64.385	10.302	20.153	1.00	34.22	Α
	ATOM	659	CD	GLN			63.340	11.169	19.459		36.88	
	ATOM	660	OE1				62.630	11.959	20.098		37.60	
	ATOM	661					63.248	11.033	18.141		35.03	
5		662	C				66.269	9.890	22.531		32.97	
3	ATOM			GLN								
	ATOM	663	0	GLN			65.857	8.768	22.825		33.19	
	ATOM	664	N	ASP			66.355	10.890	23.398		34.27	
	ATOM	665	CA	ASP	Α	151	65.847	10.771	24.753	1.00	35.77	Α
	ATOM	666	СВ	ASP	Α	151	66.957	10.933	25.796	1.00	35.66	Α
10	ATOM	667	CG	ASP	Α	151	67.760	12.194	25.604	1.00	38.11	Α
	ATOM	668	OD1	ASP	Α	151	67.172	13.216	25.195	1.00	39.31	Α
	ATOM	669		ASP			68.982	12.167	25.879		41.03	
	ATOM	670	C	ASP			64.823	11.904	24.838		36.64	
	ATOM	671	0	ASP			64.401	12.428	23.803		36.42	
15												
15	ATOM	672	N	ASP			64.427	12.301	26.041		38.18	
	ATOM	673	CA	ASP			63.427	13.357	26.171		39.81	
	ATOM	674	СВ	ASP			63.022	13.534	27.637		44.46	
	ATOM	675	CG	ASP	Α	152	62.291	12.324	28.186		50.02	
	ATOM	676	OD1	ASP	Α	152	61.313	11.876	27.541	1.00	52.36	Α
20	ATOM	677	OD2	ASP	Α	152	62.689	11.822	29.263	1.00	52.75	Α
	ATOM	678	С	ASP	Α	152	63.822	14.709	25.594	1.00	37.45	Α
	ATOM	679	0	ASP			62.988	15.408	25.026		36.81	
	ATOM	680	N	GLU			65.091	15.077	25.708		35.46	
	ATOM	681	CA	GLU			65.501	16.378	25.211		33.50	
25									26.354		36.16	
25	ATOM	682	CB	GLU			66.132	17.174				
	ATOM	683	CG	GLU			65.389	17.065	27.687		37.72	
	ATOM	684	CD	GLU			65.657	15.753	28.402		37.23	
	ATOM	685	OE 1	GLU	Α	153	65.063	15.530	29.479	0.00	37.39	Α
	ATOM	686	OE2	GLU	Α	153	66.464	14.947	27.893	0.00	37.39	Α
30	ATOM	687	С	GLU	Α	153	66.432	16.425	23.995	1.00	31.79	Α
	ATOM	688	0	GLU	Α	153	66.498	17.451	23.323	1.00	30.80	Α
	ATOM	689	N	LYS			67.131	15.334	23.691		30.35	
	ATOM	690	CA	LYS			68.069	15.357	22.569		28.14	
	ATOM	691	CB	LYS			69.505	15.358	23.099		27.32	
35		692		LYS			69.853	16.503	24.026		29.91	
33	ATOM		CG									
	ATOM	693	CD	LYS			71.234	16.302	24.648		30.14	
	ATOM	694	CE	LYS			71.606	17.450	25.592		32.52	
	ATOM	695	NZ	LYS			72.780	17.121	26.469		31.90	
	ATOM	696	С	LYS	Α	154	67.967	14.261	21.515	1.00	26.36	Α
40	ATOM	697	0	LYS	Α	154	67.517	13.145	21.781	1.00	23.71	Α
	ATOM	698	N	LEU	Α	155	68.413	14.610	20.311	1.00	24.76	Α
	ATOM	699	CA	LEU	Α	155	68.462	13.691	19.178	1.00	23.29	Α
	ATOM	700	СВ	LEU			68.012	14.382	17.891		22.72	
	ATOM	701	CG	LEU			66.588	14.916	17.739		24.25	
45	ATOM	702		LEU			66.441	15.489	16.329		24.62	
73		703		LEU			65.576	13.798	17.965		23.10	
	ATOM											
	ATOM	704	С	LEU			69.939	13.325	19.022		21.93	
	ATOM	705	0	LEU			70.812	14.167	19.233		20.17	
	ATOM	706	N	TYR			70.227	12.088	18.647		19.72	
50	ATOM	707	CA	TYR	Α	156	71.617	11.693	18.462	1.00	20.11	Α
	ATOM	708	CB	TYR	Α	156	72.061	10.703	19.540	1.00	20.01	Α
	ATOM	709	CG	TYR	Α	156	71.885	11.172	20.963	1.00	20.98	Α
	ATOM	710	CD1	TYR	Α	156	70.619	11.313	21.520	1.00	22.18	Α
	ATOM	711		TYR			70.457	11.724	22.850		25.21	
55	ATOM	712		TYR			72.991	11.449	21.762		21.38	
55	ATOM	713		TYR			72.843	11.859	23.086		25.12	
		714										
	ATOM		CZ	TYR			71.576	11.995	23.622		24.83	
	ATOM	715	OH	TYR			71.431	12.410	24.923		25.97	
	ATOM	716	С	TYR	А	T20	71.792	11.033	17.108	T.00	20.02	А

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	ATOM	717	0	TYR			70.959	10.231	16.704		22.19	
	ATOM	718	N	PHE	Α	157	72.860	11.385	16.399	1.00	19.17	Α
	ATOM	719	CA	PHE	Α	157	73.140	10.769	15.114	1.00	18.65	Α
	ATOM	720	СВ	PHE	Α	157	73.071	11.780	13.969	1.00	21.02	Α
5	ATOM	721	CG	PHE	Α	157	71.719	12.411	13.791	1.00	25.64	Δ
-	ATOM	722		PHE			70.558	11.724	14.135		27.84	
	ATOM	723		PHE			71.603	13.695	13.267		27.19	
	ATOM	724	CE1	PHE			69.301	12.310	13.964		28.87	
	ATOM	725	CE2	PHE	Α	157	70.350	14.288	13.091	1.00	28.27	Α
10	ATOM	726	CZ	PHE	Α	157	69.200	13.595	13.442	1.00	26.64	Α
	ATOM	727	С	PHE	Α	157	74.543	10.212	15.204	1.00	19.60	Α
	ATOM	728	0	PHE			75.489	10.952	15.467		19.26	
	ATOM	729	N	GLY			74.668	8.902	15.010		19.26	
	ATOM	730	CA	GLY			75.972	8.265	15.063		18.63	
1.5												
15	ATOM	731	С	GLY			76.615	8.309	13.693		16.84	
	ATOM	732	0	GLY			76.160	7.646	12.772		15.29	
	ATOM	733	N	LEU	Α	159	77.677	9.096	13.567		18.10	
	ATOM	734	CA	LEU	Α	159	78.386	9.263	12.302	1.00	17.32	Α
	ATOM	735	СВ	LEU	Α	159	78.502	10.753	11.984	1.00	16.80	Α
20	ATOM	736	CG	LEU	Α	159	77.161	11.485	12.068	1.00	18.21	Α
	ATOM	737	CD1	LEU	Α	159	77.376	12.992	12.058	1.00	15.34	Α
	ATOM	738		LEU			76.280	11.036	10.906		14.27	
	ATOM	739	C	LEU			79.780	8.665	12.375		18.27	
		740	0				80.338	8.518	13.465		18.92	
25	ATOM			LEU								
25	ATOM	741	N	SER			80.343	8.320	11.220		16.88	
	ATOM	742	CA	SER			81.691	7.770	11.194		19.02	
	ATOM	743	СВ	SER			82.086	7.362	9.771		20.02	
	ATOM	744	OG	SER	Α	160	81.866	8.421	8.864	1.00	25.88	Α
	ATOM	745	С	SER	Α	160	82.655	8.831	11.724	1.00	18.34	Α
30	ATOM	746	0	SER	Α	160	82.413	10.032	11.588	1.00	17.84	Α
	ATOM	747	N	TYR	Α	161	83.743	8.384	12.335	1.00	17.11	Α
	ATOM	748	CA	TYR			84.723	9.300	12.901		19.21	
	ATOM	749	СВ	TYR			85.146	8.802	14.293		19.37	
	ATOM	750	CG	TYR			86.269	9.582	14.944		22.52	
35		751					86.276				21.17	
33	ATOM		CD1	TYR				10.978	14.929			
	ATOM	752	CE1	TYR			87.283	11.703	15.559		18.10	
	ATOM	753	CD2	TYR			87.313	8.923	15.612		21.92	
	ATOM	754	CE2	TYR	A	161	88.330	9.647	16.252	1.00	20.10	Α
	ATOM	755	CZ	TYR	Α	161	88.301	11.039	16.220	1.00	20.24	Α
40	ATOM	756	OH	TYR	Α	161	89.266	11.776	16.873	1.00	20.31	Α
	ATOM	757	С	TYR	Α	161	85.934	9.459	11.997	1.00	20.13	Α
	ATOM	758	0	TYR	Α	161	86.621	8.491	11.675	1.00	21.97	Α
	ATOM	759	N	ALA			86.182	10.686	11.571		19.13	
	ATOM	760	CA	ALA			87.320	10.969	10.717		20.60	
45	ATOM	761	СВ	ALA			86.907	11.919	9.592		21.18	
7.7		762	C				88.375		11.604		21.36	
	ATOM			ALA				11.617				
	ATOM	763	0	ALA			88.391	12.835	11.752		20.74	
	ATOM	764	N	LYS			89.237	10.787	12.195		21.80	
	ATOM	765	CA	LYS	Α	163	90.294	11.232	13.102		25.38	
50	ATOM	766	СВ	LYS	Α	163	91.315	10.109	13.332	1.00	30.51	Α
	ATOM	767	CG	LYS	Α	163	90.874	8.987	14.251	1.00	38.24	Α
	ATOM	768	CD	LYS	Α	163	92.000	7.970	14.456	1.00	43.14	Α
	ATOM	769	CE	LYS	Α	163	91.556	6.794	15.342		46.63	
	ATOM	770	NΖ	LYS			91.252	7.200	16.752		47.21	
55	ATOM	771	C	LYS			91.082	12.482	12.719		25.07	
55		772		LYS			91.276	13.373			25.50	
	ATOM		O M						13.541			
	ATOM	773	N	ASN			91.540	12.549	11.477		25.06	
	ATOM	774	CA	ASN			92.363	13.668	11.054		26.04	
	ATOM	775	СВ	ASN	А	164	93.115	13.278	9.787	T.00	26.02	А

	7 000	776	CC	7 (7) 17 7	161	04 062	10 100	10 022	1 00 20 07 7
	ATOM	776	CG	ASN A		94.062	12.120	10.033	1.00 29.07 A
	ATOM	777		ASN A		94.854	12.155	10.969	1.00 30.18 A
	ATOM	778	ND2	ASN A	164	93.979	11.089	9.207	1.00 32.14 A
	ATOM	779	С	ASN A	164	91.725	15.040	10.915	1.00 25.35 A
5	ATOM	780	0	ASN A	164	92.416	16.021	10.640	1.00 26.51 A
	ATOM	781	N	GLY A	165	90.419	15.122	11.116	1.00 23.92 A
	ATOM	782	CA	GLY A		89.761	16.413	11.043	1.00 24.35 A
	ATOM	783	C	GLY A		89.663	17.123	9.704	1.00 23.94 A
		784	0					8.643	1.00 25.49 A
1.0	ATOM			GLY A		89.632	16.501		
10	ATOM	785	N	GLU A		89.623	18.449	9.773	1.00 23.07 A
	ATOM	786	CA	GLU A		89.467	19.301	8.602	1.00 23.26 A
	MOTA	787	СВ	GLU A	166	89.164	20.739	9.036	1.00 23.73 A
	ATOM	788	CG	GLU A	166	88.271	20.875	10.257	1.00 27.31 A
	ATOM	789	CD	GLU A	166	87.812	22.302	10.474	1.00 29.74 A
15	ATOM	790	OE 1	GLU A	166	88.586	23.221	10.130	1.00 30.87 A
	ATOM	791	OE2			86.686	22.510	10.989	1.00 29.80 A
	ATOM	792	C	GLU A		90.612	19.354	7.602	1.00 24.47 A
	ATOM	793	0	GLU A		91.786	19.473	7.968	1.00 24.85 A
• •	ATOM	794	N	LEU A		90.251	19.287	6.328	1.00 23.47 A
20	ATOM	795	CA	LEU A		91.228	19.393	5.262	1.00 24.00 A
	ATOM	796	СВ	LEU A	167	90.528	19.369	3.901	1.00 22.48 A
	ATOM	797	CG	LEU A	167	91.373	19.759	2.679	1.00 23.87 A
	ATOM	798	CD1	LEU A	167	92.583	18.846	2.563	1.00 20.03 A
	ATOM	799	CD2	LEU A		90.516	19.680	1.418	1.00 22.08 A
25	ATOM	800	С	LEU A		91.943	20.732	5.448	1.00 24.82 A
23	ATOM	801	0	LEU A		93.138	20.858	5.165	1.00 24.59 A
	ATOM	802	N	LEU A		91.206	21.731	5.927	1.00 24.43 A
	ATOM	803	CA	LEU A		91.784	23.055	6.150	1.00 28.25 A
	ATOM	804	СВ	LEU A		90.746	24.009	6.747	1.00 27.44 A
30	ATOM	805	CG	LEU A	168	91.310	25.395	7.090	1.00 28.57 A
	MOTA	806	CD1	LEU A	168	91.624	26.150	5.809	1.00 28.11 A
	ATOM	807	CD2	LEU A	168	90.312	26.174	7.921	1.00 29.97 A
	ATOM	808	С	LEU A	168	92.999	23.014	7.074	1.00 28.43 A
	ATOM	809	0	LEU A	168	93.952	23.760	6.882	1.00 30.21 A
35	ATOM	810	N	LYS A		92.958	22.152	8.081	1.00 30.23 A
55	ATOM	811	CA	LYS A		94.072	22.050	9.008	1.00 33.52 A
		812	CB	LYS A		93.821			1.00 35.32 A
	ATOM						20.955	10.046	
	ATOM	813	CG	LYS A		94.972	20.784	11.033	1.00 40.43 A
	ATOM	814	CD	LYS A		94.808	19.562	11.943	1.00 41.43 A
40	ATOM	815	CE	LYS A		95.047	18.261	11.186	1.00 42.67 A
	ATOM	816	NZ	LYS A	169	95.057	17.068	12.096	1.00 43.84 A
	ATOM	817	С	LYS A	169	95.329	21.718	8.228	1.00 34.58 A
	MOTA	818	0	LYS A	169	96.377	22.333	8.421	1.00 35.58 A
	ATOM	819	N	TYR A	170	95.219	20.739	7.339	1.00 34.55 A
45	ATOM	820	CA	TYR A		96.357	20.328	6.539	1.00 35.07 A
	ATOM	821	СВ	TYR A		96.018	19.047	5.790	1.00 35.72 A
	ATOM	822	CG	TYR A		96.050	17.869	6.716	1.00 37.48 A
	ATOM	823		TYR A		97.256	17.250	7.040	1.00 39.42 A
.	ATOM	824		TYR A		97.313	16.230	7.987	1.00 40.93 A
50	ATOM	825		TYR A		94.895	17.435	7.355	1.00 38.83 A
	MOTA	826	CE2	TYR A	170	94.937	16.417	8.303	1.00 41.76 A
	ATOM	827	CZ	TYR A	170	96.149	15.821	8.615	1.00 42.18 A
	ATOM	828	OH	TYR A	170	96.196	14.827	9.563	1.00 45.30 A
	ATOM	829	С	TYR A		96.823	21.404	5.585	1.00 35.67 A
55	ATOM	830	0	TYR A		97.999	21.465	5.248	1.00 35.28 A
22	ATOM	831		ILE A		95.904	22.260	5.154	1.00 35.20 A 1.00 36.78 A
			N						
	ATOM	832	CA	ILE A		96.272	23.333	4.252	1.00 38.95 A
	ATOM	833	СВ	ILE A		95.032	24.048	3.682	1.00 39.15 A
	ATOM	834	CG2	ILE A	171	95.452	25.329	2.960	1.00 38.11 A

	MOTA	835	CG1	ILE A	A	171	94.296	23.113	2.718		37.57 A
	ATOM	836	CD1	ILE 2	A	171	93.041	23.712	2.116	1.00	37.48 A
	ATOM	837	С	ILE A			97.146	24.338	4.990		41.33 A
_	ATOM	838	0	ILE A			98.173	24.765	4.466		42.36 A
5	MOTA	839	N	ARG I			96.748	24.713	6.203		42.79 A
	ATOM	840	CA	ARG I	A	172	97.541	25.662	6.981	1.00	44.62 A
	ATOM	841	СВ	ARG Z	A	172	96.809	26.103	8.253	1.00	46.82 A
	ATOM	842	CG	ARG A			95.492	26.828	8.033		50.73 A
10	ATOM	843	CD	ARG I			95.124	27.643	9.271		53.80 A
10	ATOM	844	NE	ARG Z	A	172	93.747	28.136	9.247	1.00	56.88 A
	ATOM	845	CZ	ARG A	A	172	93.183	28.766	8.218	1.00	57.65 A
	ATOM	846	NH1	ARG Z	A.	172	93.873	28.989	7.104	1.00	57.71 A
	ATOM	847		ARG Z			91.923	29.176	8.305		56.95 A
							98.856		7.383		44.41 A
	ATOM	848	С	ARG A				25.015			
15	MOTA	849	0	ARG Z			99.927	25.587	7.186		45.16 A
	MOTA	850	N	LYS Z	A	173	98.759	23.817	7.949	1.00	44.01 A
	ATOM	851	CA	LYS Z	Α	173	99.923	23.069	8.398	1.00	42.99 A
	ATOM	852	СВ	LYS A			99.538	21.616	8.667		44.20 A
20	ATOM	853	CG	LYS A			100.721	20.689	8.908		45.81 A
20	MOTA	854	CD	LYS Z	A	173	100.272	19.238	8.987		45.28 A
	MOTA	855	CE	LYS Z	A	173	101.457	18.296	9.120	0.00	45.43 A
	ATOM	856	NZ	LYS Z	Α	173	101.028	16.870	9.146	0.00	45.35 A
	ATOM	857	С	LYS Z			101.081	23.108	7.412	1.00	43.20 A
		858	0	LYS A			102.220	23.366	7.805		43.49 A
2.5	ATOM										
25	ATOM	859	N	ILE 2			100.802	22.867	6.133		41.97 A
	MOTA	860	CA	ILE A	A	174	101.871	22.859	5.136	1.00	40.74 A
	ATOM	861	СВ	ILE A	Α	174	101.874	21.536	4.336	1.00	40.61 A
	ATOM	862	CG2	ILE A	Α	174	101.897	20.352	5.297	1.00	41.39 A
	ATOM	863	CG1	ILE 2			100.638	21.448	3.442		40.75 A
20											
30	ATOM	864	CD1	ILE A			100.680	20.276	2.487		40.45 A
	MOTA	865	С	ILE Z			101.882	24.024	4.149		39.97 A
	MOTA	866	0	ILE 2	A	174	102.675	24.033	3.209	1.00	38.15 A
	MOTA	867	N	GLY Z	A	175	101.007	25.004	4.359	1.00	40.09 A
	ATOM	868	CA	GLY Z			100.969	26.156	3.473	1.00	39.94 A
35	ATOM	869	C	GLY Z			100.151	25.960	2.211		39.87 A
33											
	ATOM	870	0	GLY A			99.152	26.646	2.005		40.53 A
	ATOM	871	N	SER A	A	176	100.586	25.043	1.354	1.00	39.28 A
	ATOM	872	CA	SER A	A	176	99.871	24.747	0.122	1.00	38.77 A
	ATOM	873	СВ	SER Z	Ą	176	100.169	25.804	-0.950	1.00	39.84 A
40	ATOM	874	OG	SER Z			101.537	25.823	-1.319		43.67 A
10	ATOM	875	C	SER A			100.265	23.353	-0.358		38.39 A
	MOTA	876	0	SER A			101.245	22.776	0.118		39.37 A
	ATOM	877	N	PHE A	A	177	99.491	22.811	-1.289	1.00	35.85 A
	ATOM	878	CA	PHE Z	A	177	99.732	21.472	-1.810	1.00	32.81 A
45	ATOM	879	СВ	PHE 2	A	177	98.401	20.770	-2.095	1.00	32.30 A
	ATOM	880	CG	PHE 2			97.645	20.344	-0.867		31.20 A
	ATOM	881		PHE 2			97.806	21.005	0.348		29.02 A
	ATOM	882	CD2	PHE 2	A	177	96.735	19.293	-0.939	1.00	30.11 A
	MOTA	883	CE1	PHE Z	A	177	97.076	20.628	1.468	1.00	27.07 A
50	ATOM	884	CE2	PHE 2	Α	177	95.998	18.910	0.181	1.00	29.70 A
	ATOM	885	CZ	PHE 2			96.170	19.580	1.385		27.57 A
	ATOM	886	С	PHE 2			100.535	21.485	-3.093		33.02 A
	ATOM	887	0	PHE 2			100.386	22.381	-3.927	1.00	30.75 A
	MOTA	888	N	ASP Z	A	178	101.379	20.471	-3.252	1.00	33.87 A
55	ATOM	889	CA	ASP Z	A	178	102.184	20.329	-4.454	1.00	33.45 A
	ATOM	890	СВ	ASP Z			103.269	19.275	-4.244		35.60 A
			CG								40.22 A
	ATOM	891		ASP Z			102.693	17.932	-3.855		
	ATOM	892		ASP Z			101.840	17.412	-4.612		42.64 A
	MOTA	893	OD2	ASP Z	A	178	103.079	17.398	-2.793	1.00	43.32 A

	ATOM	894	C	ASP	Α	178	101.195	19.859	-5.519	1.00	32.50	Α
	ATOM	895	0	ASP	Α	178	99.999	19.723	-5.245	1.00	30.51	Α
	ATOM	896	N	GLU	Α	179	101.684	19.584	-6.720	1.00	31.46	Α
	ATOM	897	CA	GLU	Α	179	100.790	19.160	-7.779	1.00	32.00	Α
5	ATOM	898	СВ	GLU	Α	179	101.480	19.291	-9.138	1.00	33.70	Α
	ATOM	899	CG	GLU	Α	179	100.666	18.711	-10.284	1.00	38.81	Α
	ATOM	900	CD	GLU			101.129	19.195	-11.646		42.71	
	ATOM	901	OE1	GLU			102.358		-11.844		43.96	
	ATOM	902	OE2	GLU			100.261		-12.523		44.44	
10	ATOM	903	С	GLU			100.189	17.766	-7.635		29.96	
	ATOM	904	0	GLU			99.023	17.564	-7.965		27.38	
	ATOM	905	N	THR			100.959	16.803	-7.141		30.09	
	ATOM	906	CA	THR			100.429	15.448	-7.007		29.75	
	ATOM	907	СВ	THR			101.583	14.416	-6.738		30.62	
15	ATOM	908		THR			101.050	13.206	-6.179		30.65	
15	ATOM	909	CG2	THR			102.615	14.991	-5.802		32.90	
	ATOM	910	C	THR			99.331	15.372	-5.935		29.43	
	ATOM	911	0	THR			98.312	14.710	-6.130		27.52	
		911	N	CYS			99.522	16.079	-4.823		29.55	
20	MOTA	913	N CA				98.535		-3.745		29.33	
20	MOTA			CYS CYS			99.156	16.091			31.47	
	ATOM	914	CB	CYS				16.681	-2.480		39.84	
	ATOM	915	SG				100.580	15.747	-1.838			
	ATOM	916	C	CYS			97.271	16.879	-4.126		28.16	
25	ATOM	917	0	CYS			96.156	16.495	-3.762		26.55	
25	ATOM	918	N	THR			97.441	17.984	-4.847		25.71	
	ATOM	919	CA	THR			96.293	18.784	-5.268		24.22	
	ATOM	920	СВ	THR			96.714	20.043	-6.066		24.45	
	ATOM	921	OG1	THR			97.515	20.901	-5.241		22.57	
• •	ATOM	922		THR			95.483	20.809	-6.537		23.42	
30	ATOM	923	С	THR			95.447	17.915	-6.184		24.78	
	ATOM	924	0	THR			94.227	17.812	-6.020		23.72	
	ATOM	925	N	ARG			96.109	17.283	-7.149		23.96	
	ATOM	926	CA	ARG			95.422	16.419	-8.096		25.38	
	ATOM	927	СВ	ARG			96.416	15.782	-9.073		24.74	
35	ATOM	928	CG	ARG	Α	183	95.740		-10.044		27.88	
	ATOM	929	CD	ARG			96.704	14.244	-11.070	1.00	30.56	Α
	ATOM	930	NE	ARG	Α	183	97.260		-11.904		34.63	
	MOTA	931	CZ	ARG	Α	183	98.502	15.756	-11.802	1.00	33.50	Α
	MOTA	932	NH1	ARG	Α	183	99.328	15.234	-10.903	1.00	31.79	Α
40	ATOM	933	NH2	ARG	Α	183	98.901	16.754	-12.579	1.00	31.24	Α
	ATOM	934	С	ARG			94.648	15.318	-7.386		24.24	
	ATOM	935	0	ARG	Α	183	93.466	15.099	-7.659	1.00	24.95	Α
	ATOM	936	N	PHE	Α	184	95.319	14.628	-6.473	1.00	23.84	Α
	ATOM	937	CA	PHE	Α	184	94.689	13.541	-5.742	1.00	23.63	Α
45	ATOM	938	СВ	PHE	А	184	95.662	12.941	-4.730	1.00	25.29	Α
	ATOM	939	CG	PHE	Α	184	95.086	11.787	-3.961	1.00	28.53	Α
	ATOM	940	CD1	PHE	Α	184	94.958	10.531	-4.556	1.00	30.34	Α
	ATOM	941	CD2	PHE	Α	184	94.620	11.964	-2.663	1.00	28.04	Α
	ATOM	942	CE1	PHE	Α	184	94.370	9.465	-3.871	1.00	29.64	Α
50	ATOM	943	CE2	PHE	Α	184	94.030	10.908	-1.969	1.00	30.28	Α
	ATOM	944	CZ	PHE	Α	184	93.904	9.654	-2.576	1.00	29.09	Α
	ATOM	945	С	PHE	Α	184	93.431	13.977	-5.003		23.55	
	ATOM	946	0	PHE			92.353	13.429	-5.219		24.05	
	ATOM	947	N	TYR			93.568	14.961	-4.124		22.27	
55	ATOM	948	CA	TYR			92.429	15.408	-3.344		21.69	
	ATOM	949	СВ	TYR			92.925	16.295	-2.200		22.66	
	ATOM	950	CG	TYR			93.539	15.447	-1.097		25.54	
	ATOM	951		TYR			92.738	14.614	-0.314		26.51	
	ATOM	952		TYR			93.290	13.738	0.620		27.53	
		_			-							-

	ATOM	953	CD2	TYR	Α	185	94.924	15.391	-0.908	1.00	28.66	Α
	ATOM	954	CE2	TYR	Α	185	95.496	14.514	0.032	1.00	29.09	Α
	ATOM	955	CZ	TYR	Α	185	94.667	13.688	0.790	1.00	29.75	А
	ATOM	956	OH	TYR			95.204	12.806	1.702		29.03	
5	ATOM	957	C	TYR			91.316	16.058	-4.167		21.02	
5												
	ATOM	958	0	TYR			90.130	15.921	-3.851		18.76	
	ATOM	959	N	THR	Α	186	91.689	16.731	-5.244		19.87	
	MOTA	960	CA	THR	Α	186	90.690	17.337	-6.102	1.00	18.89	Α
	ATOM	961	СВ	THR	Α	186	91.344	18.170	-7.200	1.00	19.73	Α
10	ATOM	962	OG1	THR			92.115	19.218	-6.603	1.00	19.38	Α
	ATOM	963	CG2	THR			90.282	18.765	-8.125		20.16	
	MOTA	964	С	THR			89.905	16.201	-6.753		19.05	
	ATOM	965	0	THR			88.675	16.244	-6.855		19.38	
	MOTA	966	N	ALA	Α	187	90.627	15.180	-7.200	1.00	18.33	Α
15	ATOM	967	CA	ALA	Α	187	89.984	14.043	-7.841	1.00	18.09	Α
	ATOM	968	СВ	ALA			91.024	13.035	-8.276	1.00	19.99	Α
	ATOM	969	С	ALA			88.986	13.402	-6.886		18.07	
											18.54	
	ATOM	970	0	ALA			87.873	13.055	-7.291			
	ATOM	971	N	GLU			89.366	13.253	-5.617		16.56	
20	ATOM	972	CA	GLU	А	188	88.446	12.660	-4.653	1.00	16.18	Α
	ATOM	973	СВ	GLU	Α	188	89.099	12.495	-3.280	1.00	15.52	Α
	ATOM	974	CG	GLU	Α	188	90.266	11.519	-3.259	1.00	20.99	Α
	ATOM	975	CD	GLU	А	188	90.297	10.636	-2.013	1.00	22.64	А
	ATOM	976		GLU			90.006	11.126	-0.899		22.95	
25	ATOM	977	OE2	GLU			90.629	9.439	-2.149		27.37	
23												
	ATOM	978	С	GLU			87.189	13.508	-4.518		15.81	
	ATOM	979	0	GLU			86.080	12.978	-4.460		15.92	
	ATOM	980	N	ILE			87.364	14.825	-4.483		16.14	
	ATOM	981	CA	ILE	Α	189	86.235	15.733	-4.346	1.00	16.66	Α
30	ATOM	982	СВ	ILE	Α	189	86.698	17.179	-4.083	1.00	16.57	Α
	ATOM	983	CG2	ILE	Α	189	85.485	18.098	-3.958	1.00	14.92	Α
	ATOM	984	CG1	ILE	Α	189	87.502	17.235	-2.784	1.00	16.19	Α
	ATOM	985	CD1	ILE			88.202	18.559	-2.547		16.78	
	ATOM	986	C	ILE			85.349	15.712	-5.580		16.29	
35	ATOM	987	0	ILE			84.123	15.667	-5.471		15.80	
33												
	ATOM	988	N	VAL			85.962	15.743	-6.755		16.44	
	ATOM	989	CA	VAL			85.186	15.704	-7.985		15.98	
	MOTA	990	СВ	VAL	Α	190	86.101	15.692	-9.229	1.00	17.23	Α
	MOTA	991	CG1	VAL	Α	190	85.280	15.380	-10.488	1.00	16.01	Α
40	ATOM	992	CG2	VAL	Α	190	86.797	17.034	-9.373	1.00	13.82	Α
	ATOM	993	С	VAL	А	190	84.351	14.433	-7.979	1.00	16.29	Α
	ATOM	994	0	VAL			83.140	14.462	-8.194		15.64	
	ATOM	995	N	SER			85.011	13.312	-7.723		18.94	
											18.50	
4.5	ATOM	996	CA	SER			84.337	12.015	-7.692			
45	MOTA	997	СВ	SER			85.357	10.914	-7.427		19.04	
	ATOM	998	OG	SER	A	191	84.712	9.680	-7.206	1.00	23.87	Α
	MOTA	999	С	SER	Α	191	83.233	11.961	-6.642	1.00	16.85	Α
	ATOM	1000	0	SER	Α	191	82.227	11.281	-6.818	1.00	18.11	Α
	ATOM	1001	N	ALA	Α	192	83.419	12.671	-5.540	1.00	17.37	Α
50	ATOM	1002	CA	ALA			82.395	12.687	-4.501		17.10	
20		1003	СВ	ALA			82.947	13.302	-3.222		17.08	
	ATOM											
	ATOM	1004	С	ALA			81.218	13.511	-5.020		18.24	
	ATOM	1005	0	ALA			80.055	13.162	-4.798		18.91	
	ATOM	1006	N	LEU	Α	193	81.524	14.597	-5.725		16.53	
55	ATOM	1007	CA	LEU	Α	193	80.483	15.453	-6.270	1.00	17.25	Α
	ATOM	1008	СВ	LEU	Α	193	81.091	16.750	-6.826		17.70	
	ATOM	1009	CG	LEU			81.537	17.738	-5.732		22.88	
	ATOM	1010		LEU			82.094	19.018	-6.348		22.13	
	ATOM	1011		LEU			80.345	18.057	-4.839		20.04	
	111 011	TO TT	OD2	UU (2 L	100	0.010	10.007	1.000	1.00	_0.01	7.7

	7) III () M	1010	a	TEST	7\	102	70 664	11 727	7 2/2	1 00	17.26	70
	ATOM	1012	C	LEU			79.664	14.737	-7.343			
	ATOM	1013	0	LEU			78.442	14.893	-7.402		15.43	
	MOTA	1014	N	GLU			80.330	13.962	-8.195		16.22	
	MOTA	1015	CA	GLU			79.612	13.232	-9.225		19.22	
5	ATOM	1016	СВ	GLU			80.564	12.405	-10.086		20.77	
	ATOM	1017	CG	GLU	Α	194	79.828	11.403	-10.978	1.00	26.27	Α
	ATOM	1018	CD	GLU	Α	194	80.756	10.667	-11.934	1.00	29.43	Α
	ATOM	1019	OE1	GLU	Α	194	81.840	10.222	-11.489	1.00	28.21	Α
	ATOM	1020	OE2	GLU	Α	194	80.392	10.532	-13.127	1.00	31.66	Α
10	ATOM	1021	С	GLU	Α	194	78.599	12.303	-8.566	1.00	19.71	Α
	ATOM	1022	0	GLU	Α	194	77.466	12.159	-9.027	1.00	18.40	Α
	ATOM	1023	N	TYR			79.012	11.672	-7.479		19.22	
	ATOM	1024	CA	TYR			78.116	10.773	-6.781		19.69	
	ATOM	1025	СВ	TYR			78.867	10.041	-5.667		21.39	
15	ATOM	1026	CG	TYR			77.975	9.143	-4.847		22.55	
13	ATOM	1027		TYR			77.596	7.881	-5.316		23.14	
	ATOM	1027		TYR			76.743	7.065	-4.577		22.98	
		1028	CD2	TYR			77.479	9.564	-3.618		21.58	
	ATOM	1029	CE2	TYR			76.625	8.755	-2.872		23.50	
20	ATOM											
20	ATOM	1031	CZ	TYR			76.263	7.512	-3.358		23.18	
	ATOM	1032	OH	TYR			75.413	6.732	-2.632		24.19	
	ATOM	1033	С	TYR			76.939	11.546	-6.172		18.80	
	ATOM	1034	0	TYR			75.782	11.164	-6.337		19.89	
	MOTA	1035	N	LEU			77.242	12.629	-5.469		15.26	
25	MOTA	1036	CA	LEU			76.210	13.430	-4.813		16.52	
	MOTA	1037	СВ	LEU			76.855	14.586	-4.038		15.67	
	MOTA	1038	CG	LEU			75.923	15.401	-3.131		19.13	
	MOTA	1039	CD1	LEU			75.555	14.571	-1.903		18.42	
	MOTA	1040	CD2	LEU	А	196	76.604	16.681	-2.689		18.50	
30	MOTA	1041	С	LEU	Α	196	75.209	13.993	-5.814	1.00	18.12	Α
	MOTA	1042	0	LEU	Α	196	73.990	13.892	-5.637	1.00	16.25	Α
	ATOM	1043	N	HIS	Α	197	75.732	14.592	-6.875	1.00	17.99	Α
	ATOM	1044	CA	HIS	Α	197	74.873	15.171	-7.878	1.00	20.69	Α
	ATOM	1045	СВ	HIS	Α	197	75.715	16.004	-8.832	1.00	19.71	Α
35	ATOM	1046	CG	HIS	Α	197	76.292	17.224	-8.190	1.00	19.55	Α
	ATOM	1047	CD2	HIS	Α	197	76.069	17.777	-6.973	1.00	18.32	Α
	ATOM	1048		HIS			77.172	18.063	-8.837		20.26	
	ATOM	1049		HIS			77.463	19.084	-8.049		20.73	
	ATOM	1050		HIS			76.806	18.935	-6.913		19.92	
40	ATOM	1051	С	HIS			74.091	14.093	-8.609		22.80	
	ATOM	1052	0	HIS			72.974	14.328	-9.068		21.91	
	ATOM	1053	N	GLY			74.672	12.903	-8.697		23.17	
	ATOM	1054	CA	GLY			73.990	11.815	-9.366		26.22	
	ATOM	1055	C	GLY			72.718	11.436	-8.631		27.16	
45	ATOM	1056	0	GLY			71.837	10.787	-9.185		27.89	
15	ATOM	1057	N	LYS			72.623	11.831	-7.369		27.84	
	ATOM	1057	CA	LYS			71.429	11.532	-6.587		28.20	
	ATOM	1059	CB	LYS			71.423	10.952	-5.227		29.35	
	ATOM	1060	CG					9.502				
50		1060		LYS LYS			72.278	8.944	-5.321		32.74	
30	ATOM		CD				72.737		-3.990		38.22	
	ATOM	1062	CE	LYS			72.600	7.424	-3.965		41.17	
	ATOM	1063	NZ	LYS			73.173	6.779	-5.185		44.70	
	ATOM	1064	С	LYS			70.542	12.765	-6.419		26.97	
	ATOM	1065	0	LYS			69.678	12.807	-5.551		28.27	
55	ATOM	1066	N	GLY			70.759	13.762	-7.269		25.62	
	MOTA	1067	CA	GLY			69.963	14.972	-7.222		24.75	
	MOTA	1068	С	GLY			70.070	15.713	-5.908		25.82	
	MOTA	1069	0	GLY			69.080	16.241	-5.401		26.10	
	ATOM	1070	N	ILE	Α	201	71.275	15.759	-5.353	1.00	25.31	Α

	ATOM	1071	CA	ILE	Α	201	71.490	16.440	-4.089	1.00	26.11 A
	ATOM	1072	CB	ILE	Α	201	71.886	15.438	-2.983	1.00	27.58 A
	ATOM	1073	CG2	ILE	Α	201	72.242	16.175	-1.704	1.00	27.99 A
	ATOM	1074	CG1	ILE			70.725	14.480	-2.719		27.89 A
5	ATOM	1075		ILE			71.068	13.366	-1.746		30.62 A
)											
	ATOM	1076	С	ILE			72.576	17.489	-4.233		25.92 A
	MOTA	1077	0	ILE	Α	201	73.599	17.269	-4.887	1.00	25.94 A
	MOTA	1078	N	ILE	Α	202	72.337	18.640	-3.627	1.00	25.04 A
	ATOM	1079	CA	ILE	Α	202	73.289	19.733	-3.680	1.00	26.57 A
10	ATOM	1080	СВ	ILE			72.640	20.990	-4.286		27.69 A
10											
	ATOM	1081	CG2	ILE			73.695	22.068	-4.516		30.47 A
	ATOM	1082	CG1	ILE			71.992	20.639	-5.625		30.89 A
	ATOM	1083	CD1	ILE	Α	202	71.083	21.736	-6.178	1.00	31.79 A
	ATOM	1084	С	ILE	Α	202	73.742	20.032	-2.252	1.00	26.14 A
15	ATOM	1085	0	ILE			72.912	20.201	-1.351		24.75 A
15	ATOM	1086	N	HIS			75.054	20.075	-2.042		25.17 A
	ATOM	1087	CA	HIS			75.585	20.362	-0.717		24.36 A
	ATOM	1088	СВ	HIS	Α	203	77.095	20.131	-0.677	1.00	23.06 A
	ATOM	1089	CG	HIS	Α	203	77.680	20.268	0.694	1.00	24.09 A
20	ATOM	1090	CD2	HIS	Α	203	77.956	21.366	1.434	1.00	22.36 A
	ATOM	1091		HIS			77.981	19.183	1.490		23.65 A
		1092		HIS				19.607			23.87 A
	ATOM						78.418		2.661		
	ATOM	1093	NE2	HIS			78.412	20.929	2.653		25.12 A
	MOTA	1094	С	HIS	Α	203	75.269	21.811	-0.330	1.00	24.71 A
25	ATOM	1095	0	HIS	Α	203	74.633	22.055	0.693	1.00	24.27 A
	ATOM	1096	N	ARG	Α	204	75.724	22.758	-1.154	1.00	25.89 A
	ATOM	1097	CA	ARG			75.490	24.199	-0.961		25.68 A
	ATOM	1098	CB	ARG			74.033	24.471	-0.596		25.57 A
	ATOM	1099	CG	ARG			73.079	24.319	-1.751		29.26 A
30	MOTA	1100	CD	ARG	Α	204	71.815	25.118	-1.509	1.00	29.86 A
	ATOM	1101	NE	ARG	Α	204	71.065	24.603	-0.373	1.00	33.90 A
	ATOM	1102	CZ	ARG	Α	204	70.021	25.219	0.170	1.00	36.01 A
	ATOM	1103		ARG			69.607	26.383	-0.322		37.08 A
				ARG							
2.5	ATOM	1104					69.387	24.668	1.197		34.14 A
35	ATOM	1105	С	ARG			76.373	24.935	0.034		26.91 A
	MOTA	1106	0	ARG	Α	204	76.210	26.144	0.243	1.00	26.29 A
	ATOM	1107	N	ASP	Α	205	77.303	24.221	0.654	1.00	26.23 A
	ATOM	1108	CA	ASP	Α	205	78.203	24.849	1.604	1.00	24.46 A
	ATOM	1109	СВ	ASP			77.557	24.909	2.990		28.25 A
40	ATOM	1110	CG	ASP			78.203	25.954	3.890		30.95 A
70											
	ATOM	1111		ASP			78.872	26.862	3.354		35.13 A
	ATOM	1112	OD2	ASP			78.034	25.880	5.127		33.48 A
	MOTA	1113	С	ASP	Α	205	79.483	24.039	1.631	1.00	24.22 A
	MOTA	1114	0	ASP	Α	205	79.998	23.676	2.685	1.00	23.62 A
45	ATOM	1115	N	LEU	Α	206	79.995	23.755	0.442	1.00	23.31 A
	ATOM	1116	CA	LEU			81.206		0.321		24.19 A
	ATOM	1117	СВ	LEU			81.311	22.406	-1.088		24.78 A
	ATOM	1118	CG	LEU			82.353	21.309	-1.285		25.24 A
	MOTA	1119	CD1	LEU	Α	206	82.075	20.173	-0.317	1.00	26.72 A
50	MOTA	1120	CD2	LEU	Α	206	82.298	20.808	-2.720	1.00	24.32 A
	ATOM	1121	С	LEU	Α	206	82.408	23.853	0.623		24.52 A
	ATOM	1122	0	LEU			82.508	24.977	0.130		24.34 A
	ATOM	1123	N	LYS			83.328	23.330	1.424		22.98 A
	ATOM	1124	CA	LYS	Α	207	84.517	24.083	1.796	1.00	23.05 A
55	ATOM	1125	СВ	LYS	А	207	84.113	25.305	2.629	1.00	21.18 A
	ATOM	1126	CG	LYS	Α	207	83.278	24.948	3.830		19.29 A
	ATOM	1127	CD	LYS			82.775	26.179	4.568		23.68 A
	ATOM	1128	CE	LYS			81.913	25.781	5.767		21.99 A
	ATOM	1129	ΝZ	LYS	А	ZU /	81.580	26.910	6.686	1.00	25.14 A

	ATOM	1130	С	LYS	Α	207	85.444	23.183	2.602	1.00	23.54 A
	ATOM	1131	0	LYS			85.014	22.169	3.144		26.04 A
	ATOM	1132	N	PRO			86.728	23.550	2.697		23.78 A
	ATOM	1133	CD			208	87.309	24.764	2.100		21.90 A
5	ATOM	1134	CA	PRO			87.754	22.801	3.429		23.64 A
3		1134					88.948	23.750	3.397		22.67 A
	ATOM		CB	PRO							
	ATOM	1136	CG	PRO			88.779	24.432	2.084		23.00 A
	ATOM	1137	С	PRO			87.393	22.390	4.859		24.47 A
	MOTA	1138	0	PRO			87.890	21.378	5.358		24.20 A
10	MOTA	1139	N	GLU	Α	209	86.541	23.176	5.514	1.00	25.33 A
	ATOM	1140	CA	GLU	Α	209	86.132	22.903	6.894	1.00	26.78 A
	ATOM	1141	СВ	GLU	Α	209	85.641	24.190	7.570	1.00	27.82 A
	ATOM	1142	CG	GLU	Α	209	86.616	25.359	7.479	1.00	34.76 A
	ATOM	1143	CD	GLU	Α	209	86.459	26.183	6.199		39.84 A
15	ATOM	1144		GLU			86.575	25.628	5.079		38.56 A
	ATOM	1145	OE2	GLU			86.219	27.405	6.322		44.97 A
	ATOM	1146	C	GLU			85.039	21.840	6.972		26.70 A
	ATOM	1147	0	GLU			84.786	21.269	8.035		29.78 A
20	ATOM	1148	N	ASN			84.395	21.583	5.841		24.55 A
20	ATOM	1149	CA	ASN			83.339	20.587	5.751		24.33 A
	ATOM	1150	СВ	ASN			82.195	21.105	4.866		27.29 A
	MOTA	1151	CG	ASN	Α	210	81.225	21.998	5.622		31.63 A
	ATOM	1152	OD1	ASN	Α	210	80.280	22.539	5.040	1.00	35.25 A
	MOTA	1153	ND2	ASN	Α	210	81.449	22.155	6.923	1.00	30.78 A
25	ATOM	1154	С	ASN	Α	210	83.885	19.289	5.158	1.00	22.61 A
	ATOM	1155	0	ASN	Α	210	83.207	18.268	5.155	1.00	19.95 A
	ATOM	1156	N			211	85.105	19.344	4.638	1.00	22.15 A
	ATOM	1157	CA			211	85.733	18.174	4.043		21.36 A
	ATOM	1158	СВ			211	86.467	18.538	2.744		20.33 A
30	ATOM	1159	CG2			211	87.167	17.315	2.180		20.04 A
50	ATOM	1160	CG1	ILE			85.475	19.089	1.719		19.57 A
	ATOM	1161					86.162	19.718	0.517		20.56 A
		1162	CDI				86.733	17.629			20.36 A
	MOTA					211			5.048		
2.5	ATOM	1163	0	ILE			87.805	18.209	5.254		21.87 A
35	ATOM	1164	N	LEU			86.377	16.510	5.670		21.03 A
	ATOM	1165	CA	LEU			87.228	15.910	6.685		20.43 A
	ATOM	1166	СВ	LEU			86.352	15.331	7.801		19.57 A
	ATOM	1167	CG	LEU	Α	212	85.270	16.281	8.347		19.01 A
	MOTA	1168	CD1	LEU	Α	212	84.543	15.613	9.494	1.00	16.54 A
40	ATOM	1169	CD2	LEU	Α	212	85.903	17.592	8.817	1.00	19.58 A
	MOTA	1170	С	LEU	Α	212	88.148	14.833	6.139	1.00	20.95 A
	ATOM	1171	0	LEU	Α	212	88.034	14.420	4.983	1.00	20.16 A
	ATOM	1172	N			213	89.069				21.07 A
	ATOM	1173	CA			213	89.991				21.58 A
45	ATOM	1174	СВ			213	91.415	13.882	6.520		21.17 A
	ATOM	1175	CG			213	91.633	14.944	5.440		21.26 A
	ATOM	1176		LEU			93.051	15.466	5.514		23.93 A
		1177		LEU			91.378		4.070		23.36 A
	ATOM					213					
50	ATOM	1178	C				89.912		7.554		22.28 A
50	ATOM	1179	0			213	89.948		8.766		23.80 A
	ATOM	1180	N	ASN			89.786		7.025		22.96 A
	ATOM	1181	CA	ASN	Α		89.718				22.83 A
	MOTA	1182	СВ	ASN		214	88.997	8.647			3.75 AC1
	ATOM	1183	CG	ASN		214	89.144	7.286			5.62 AC1
55	ATOM	1184	OD1	ASN		214	90.212	6.673	7.713 0	.50 25	5.34 AC1
	ATOM	1185	ND2	ASN		214	88.066	6.803	8.363 0	.50 26	5.41 AC1
	ATOM	1186	С	ASN	Α	214	91.151				23.68 A
	ATOM	1187	0			214			7.716		
	ATOM	1188	N	GLU			91.291	8.379	9.119		25.06 A
							22.232				

	ATOM	1189	CA	GLU	Α	215	92.603	7.901	9.545	1.00 26.20 A
	ATOM	1190	СВ	GLU	Α	215	92.453	6.669	10.435	1.00 26.19 A
	ATOM	1191	CG	GLU			93.770	6.153	10.985	1.00 29.08 A
_	MOTA	1192	CD	GLU			93.589	4.963	11.907	0.00 28.21 A
5	MOTA	1193	OE1	GLU	Α	215	93.064	3.927	11.449	0.00 28.42 A
	ATOM	1194	OE2	GLU	Α	215	93.973	5.065	13.092	0.00 28.42 A
	ATOM	1195	С	GLU	Α	215	93.532	7.566	8.385	1.00 26.12 A
	ATOM	1196	0	GLU			94.746	7.743	8.487	1.00 29.48 A
	MOTA	1197	N	ASP			92.976	7.070	7.287	1.00 25.52 A
10	ATOM	1198	CA	ASP	Α	216	93.798	6.728	6.133	1.00 25.79 A
	ATOM	1199	СВ	ASP		216	93.164	5.564	5.376 0	.50 27.09 AC1
	ATOM	1200	CG	ASP		216	93.450	4.231		.50 29.11 AC1
	ATOM	1201		ASP		216	93.206	4.098		.50 31.09 AC1
	MOTA	1202		ASP		216	93.921	3.315		.50 31.52 AC1
15	ATOM	1203	С	ASP	Α	216	94.034	7.896	5.173	1.00 24.88 A
	ATOM	1204	0	ASP	Α	216	94.586	7.719	4.094	1.00 26.27 A
	ATOM	1205	N	MET	Α	217	93.615	9.087	5.578	1.00 25.04 A
	ATOM	1206	CA	MET			93.789	10.301	4.792	1.00 24.86 A
• •	MOTA	1207	СВ	MET			95.270	10.503	4.454	1.00 28.81 A
20	ATOM	1208	CG	MET	Α	217	96.139	10.834	5.676	1.00 29.66 A
	ATOM	1209	SD	MET	Α	217	95.577	12.323	6.551	1.00 34.79 A
	ATOM	1210	CE	MET	Α	217	96.130	13.598	5.411	1.00 30.61 A
	ATOM	1211	C	MET			92.942	10.437	3.528	1.00 24.93 A
										1.00 24.33 A
	MOTA	1212	0	MET			93.277	11.215	2.629	
25	ATOM	1213	N	HIS			91.855	9.678	3.450	1.00 21.48 A
	ATOM	1214	CA	HIS	Α	218	90.947	9.799	2.319	1.00 21.72 A
	ATOM	1215	СВ	HIS	Α	218	90.325	8.444	1.963	1.00 21.43 A
	ATOM	1216	CG	HIS	Δ	218	91.225	7.578	1.138	1.00 24.55 A
	ATOM	1217		HIS			91.951	6.478	1.458	1.00 23.50 A
20										
30	MOTA	1218		HIS			91.522	7.860	-0.179	1.00 23.64 A
	MOTA	1219	CE1	HIS	Α	218	92.392	6.975	-0.633	1.00 21.12 A
	ATOM	1220	NE2	HIS	Α	218	92.670	6.128	0.340	1.00 22.96 A
	ATOM	1221	С	HIS	Α	218	89.891	10.785	2.812	1.00 20.49 A
	ATOM	1222	0	HIS			89.683	10.911	4.018	1.00 20.60 A
25										
35	ATOM	1223	N	ILE			89.231	11.488	1.897	1.00 18.82 A
	ATOM	1224	CA	ILE			88.244	12.473	2.306	1.00 17.27 A
	ATOM	1225	CB	ILE	Α	219	87.914	13.487	1.178	1.00 15.59 A
	ATOM	1226	CG2	ILE	Α	219	89.175	14.201	0.718	1.00 14.62 A
	MOTA	1227	CG1	ILE	Δ	219	87.252	12.769	0.006	1.00 16.04 A
40	ATOM	1228	CD1	ILE			86.458	13.685	-0.888	1.00 15.29 A
40										
	MOTA	1229	С	ILE			86.934	11.885	2.772	1.00 17.64 A
	ATOM	1230	0	ILE	Α	219	86.564	10.774	2.402	1.00 18.93 A
	ATOM	1231	N	GLN	Α	220	86.240	12.658	3.597	1.00 19.19 A
	ATOM	1232	CA	GLN	Α	220	84.933	12.293	4.119	1.00 21.50 A
45	ATOM	1233	СВ	GLN			85.061	11.585	5.475	1.00 23.96 A
15										
	MOTA	1234	CG	GLN			85.583	10.151	5.334	1.00 29.77 A
	ATOM	1235	CD	GLN	Α	220	84.945	9.182	6.319	1.00 33.77 A
	ATOM	1236	OE1	GLN	Α	220	85.257	9.188	7.513	1.00 37.87 A
	ATOM	1237	NE2	GLN	Α	220	84.040	8.347	5.821	1.00 34.29 A
50	ATOM	1238	С	GLN			84.158	13.599	4.240	1.00 21.53 A
50										
	ATOM	1239	0	GLN			84.367		5.166	1.00 22.54 A
	MOTA	1240	N			221	83.284	13.833	3.270	1.00 19.63 A
	MOTA	1241	CA	ILE	Α	221	82.498	15.054	3.234	1.00 19.30 A
	ATOM	1242	СВ	ILE	Α	221	82.055	15.366	1.785	1.00 20.41 A
55	ATOM	1243		ILE			81.237	16.639	1.738	1.00 19.39 A
55										
	ATOM	1244		ILE			83.290		0.900	1.00 19.44 A
	MOTA	1245		ILE			82.977	15.802		1.00 17.44 A
	MOTA	1246	С	ILE	Α	221	81.284	14.951	4.141	1.00 18.36 A
	MOTA	1247	0	ILE	Α	221	80.627	13.911	4.204	1.00 15.98 A

		4040			_			4.6.004		4 00	40 50 -
	MOTA	1248	N	THR			80.995	16.024	4.864		19.59 A
	ATOM	1249	CA	THR	Α	222	79.844	16.008	5.753	1.00	22.76 A
	ATOM	1250	СВ	THR	Α	222	80.218	15.420	7.126	1.00	23.86 A
	ATOM	1251	OG1	THR	Α	222	79.019	15.145	7.863	1.00	28.20 A
5	ATOM	1252	CG2	THR			81.105	16.380	7.908		23.65 A
5				THR			79.179	17.370			23.55 A
	ATOM	1253	С						5.933		
	ATOM	1254	0	THR			79.505	18.334	5.229		25.65 A
	MOTA	1255	N	ASP	Α	223	78.248	17.427	6.881	1.00	24.38 A
	ATOM	1256	CA	ASP	Α	223	77.449	18.611	7.202	1.00	25.25 A
10	ATOM	1257	СВ	ASP	Α	223	78.303	19.865	7.422		26.12 A
	ATOM	1258	CG	ASP			77.538	20.962	8.175		29.92 A
	ATOM	1259		ASP			76.288	20.876	8.278		31.91 A
	MOTA	1260	OD2	ASP			78.177	21.911	8.671		32.94 A
	ATOM	1261	С	ASP	Α	223	76.461	18.882	6.080	1.00	25.61 A
15	ATOM	1262	0	ASP	Α	223	76.693	19.744	5.227	1.00	25.81 A
	ATOM	1263	N	PHE	Α	224	75.358	18.139	6.098		25.18 A
	ATOM	1264	CA	PHE			74.310	18.266	5.096		26.75 A
	ATOM	1265	СВ	PHE			73.860	16.879	4.635		27.24 A
	ATOM	1266	CG	PHE			74.857	16.189	3.753		28.10 A
20	MOTA	1267	CD1	PHE	Α	224	74.889	16.450	2.388	1.00	29.12 A
	ATOM	1268	CD2	PHE	Α	224	75.790	15.313	4.291	1.00	28.67 A
	ATOM	1269	CE1	PHE	Δ	224	75.841	15.847	1.567		30.28 A
		1270	CE2	PHE			76.745	14.706	3.482		31.49 A
	ATOM										
	MOTA	1271	CZ	PHE			76.770	14.973	2.117		30.54 A
25	ATOM	1272	С	PHE	Α	224	73.124	19.038	5.632	1.00	27.73 A
	MOTA	1273	0	PHE	Α	224	72.005	18.895	5.140	1.00	27.84 A
	ATOM	1274	N	GLY	Α	225	73.378	19.862	6.643	1.00	29.36 A
	ATOM	1275	CA	GLY	Δ	225	72.319	20.656	7.235	1.00	30.10 A
	ATOM	1276	C	GLY			71.825	21.741	6.297		31.32 A
20											
30	ATOM	1277	0	GLY			70.714	22.248	6.451		32.90 A
	ATOM	1278	N	THR	Α	226	72.640	22.091	5.311	1.00	29.95 A
	ATOM	1279	CA	THR	Α	226	72.261	23.132	4.365	1.00	32.06 A
	ATOM	1280	СВ	THR	Α	226	73.381	24.167	4.226	1.00	33.35 A
	ATOM	1281	OG1	THR			74.454	23.608	3.455		35.74 A
35	ATOM	1282	CG2	THR			73.920	24.542	5.593		34.02 A
33											
	ATOM	1283	С	THR			71.979	22.551	2.983		31.11 A
	ATOM	1284	0	THR			71.801	23.288	2.012		30.89 A
	ATOM	1285	N	ALA	Α	227	71.938	21.230	2.899	1.00	30.02 A
	ATOM	1286	CA	ALA	Α	227	71.714	20.566	1.624	1.00	32.20 A
40	ATOM	1287	СВ	ALA	Α	227	71.906	19.057	1.770	1.00	29.19 A
	ATOM	1288	С	ALA	Δ	227	70.345	20.865	1.045		32.77 A
	ATOM	1289	0	ALA			69.431	21.269	1.761		34.17 A
	ATOM	1290	N	ALA			70.229	20.684	-0.266		33.18 A
	ATOM	1291	CA	ALA			68.980	20.902	-0.982		34.43 A
45	ATOM	1292	СВ	ALA	Α	228	69.079	22.146	-1.861		32.03 A
	ATOM	1293	С	ALA	Α	228	68.742	19.674	-1.846	1.00	35.25 A
	ATOM	1294	0	ALA	Α	228	69.612	19.284	-2.622	1.00	36.70 A
	ATOM	1295	N	VAL			67.578	19.056	-1.698		36.21 A
				VAL			67.246				
50	ATOM	1296	CA					17.876	-2.488		37.95 A
50	ATOM	1297	СВ	VAL			66.438	16.857	-1.674		37.37 A
	ATOM	1298	CG1	VAL	Α	229	66.192	15.609	-2.506	1.00	35.62 A
	ATOM	1299	CG2	VAL	Α	229	67.176	16.522	-0.394	1.00	36.39 A
	ATOM	1300	С	VAL	Α	229	66.393	18.341	-3.649	1.00	40.15 A
	ATOM	1301	0	VAL			65.353	18.965	-3.446		39.20 A
55											
55	ATOM	1302	N	LEU			66.836	18.044	-4.865		43.75 A
	MOTA	1303	CA	LEU			66.105	18.455	-6.054		48.04 A
	ATOM	1304	СВ	LEU			67.039	18.473	-7.258		48.59 A
	ATOM	1305	CG	LEU	Α	230	68.123	19.552	-7.212		50.35 A
	ATOM	1306	CD1	LEU	Α	230	69.118	19.312	-8.326	1.00	50.62 A

	ATOM	1307	CD2	LEU	7\	230	67.488	20.932	-7.330	1 00	50.11	7\
				LEU								
	ATOM	1308	C				64.905	17.569	-6.346		51.38	
	ATOM	1309	0	LEU			64.929	16.364	-6.095		51.84	
-	ATOM	1310	N	SER			63.854	18.190	-6.872		56.03	
5	ATOM	1311	CA	SER			62.616	17.502	-7.224		60.24	
	MOTA	1312	СВ	SER			61.528	17.806	-6.186		60.77	
	MOTA	1313	OG	SER			61.222	19.192	-6.150	1.00		
	ATOM	1314	С			231	62.115	17.894	-8.622		62.65	
	ATOM	1315	0	SER			61.527	17.068	-9.326	1.00	63.42	Α
10	MOTA	1316	N	PRO	Α	232	62.334	19.161	-9.040	1.00	64.66	Α
	MOTA	1317	CD	PRO	Α	232	62.903	20.298	-8.289	1.00	64.95	Α
	ATOM	1318	CA	PRO	Α	232	61.882	19.604	-10.367	1.00	65.69	Α
	ATOM	1319	СВ	PRO	Α	232	62.409	21.037	-10.450	1.00	65.77	Α
	ATOM	1320	CG	PRO	Α	232	62.341	21.493	-9.031	1.00	65.52	Α
15	ATOM	1321	С	PRO	Α	232	62.408	18.731	-11.505	1.00	66.28	Α
	ATOM	1322	0	PRO	Α	232	62.858	19.241	-12.532	1.00	66.55	Α
	ATOM	1323	N	ALA			65.927	26.021	-3.995	1.00	92.57	А
	ATOM	1324	CA	ALA			67.330	26.100	-3.606		92.64	
	ATOM	1325	СВ	ALA			68.187	25.262	-4.558		92.15	
20	ATOM	1326	C	ALA			67.769	27.558	-3.640		92.34	
	ATOM	1327	0	ALA			68.683	27.930	-4.373		92.47	
	ATOM	1328	N	ASN			67.108	28.379	-2.833		91.92	
	ATOM	1329	CA	ASN			67.396	29.809	-2.767		91.12	
	ATOM	1330	CB	ASN			66.374	30.566	-3.617		92.32	
25	ATOM	1331	CG	ASN			64.947	30.084	-3.378		93.20	
23	ATOM	1331		ASN			64.471	30.064	-2.244		93.46	
		1333					64.261	29.697	-2.244 -4.452		94.00	
	ATOM			ASN								
	ATOM	1334	C	ASN			67.334	30.332	-1.335		89.78	
20	ATOM	1335	0	ASN			67.766	31.453	-1.053		89.80	
30	ATOM	1336	N	ALA			66.787	29.515	-0.441		88.16	
	ATOM	1337	CA	ALA			66.624	29.891	0.955		86.55	
	ATOM	1338	С	ALA			67.901	29.893	1.792		84.55	
	ATOM	1339	0	ALA			67.865	30.268	2.961		84.76	
	MOTA	1340	СВ	ALA			65.583	28.978	1.623		88.01	
35	MOTA	1341	N	PHE			69.028	29.494	1.216		82.28	
	MOTA	1342	CA	PHE			70.264	29.483	1.993		79.83	
	MOTA	1343	СВ	PHE			70.718	28.046	2.282		79.60	
	MOTA	1344	CG	PHE	Α	242	71.980	27.962	3.100	1.00	79.10	Α
	ATOM	1345	CD1	PHE			72.024	28.483	4.388	1.00	79.45	Α
40	MOTA	1346	CD2	PHE	Α	242	73.131	27.392	2.571	1.00	79.42	Α
	MOTA	1347	CE1	PHE	Α	242	73.202	28.442	5.143	1.00	79.29	Α
	MOTA	1348	CE2	PHE	Α	242	74.314	27.345	3.317	1.00	80.20	Α
	MOTA	1349	CZ	PHE	Α	242	74.348	27.872	4.605	1.00	79.98	Α
	ATOM	1350	С	PHE	Α	242	71.402	30.231	1.322	1.00	77.56	Α
45	ATOM	1351	0	PHE	Α	242	71.347	30.524	0.130	1.00	78.59	Α
	ATOM	1352	N	VAL	Α	243	72.440	30.529	2.098	1.00	73.76	Α
	ATOM	1353	CA	VAL	Α	243	73.595	31.238	1.579	1.00	70.34	Α
	ATOM	1354	СВ	VAL	Α	243	73.864	32.515	2.405	1.00	71.71	Α
	ATOM	1355	CG1	VAL	Α	243	75.087	33.238	1.859	1.00	71.29	Α
50	ATOM	1356		VAL			72.638	33.425	2.376		71.41	
	ATOM	1357	С	VAL			74.851	30.362	1.581		66.69	
	ATOM	1358	0	VAL			75.232	29.802	0.552		66.50	
	ATOM	1359	N	GLY			75.496	30.245	2.737		62.34	
	ATOM	1360	CA	GLY			76.708	29.444	2.829		56.48	
55	ATOM	1361	CA	GLY			77.889	30.327	3.168		52.17	
55	ATOM	1361	0	GLY			77.769	31.547	3.136		52.14	
		1362		THR			79.031	29.733	3.490		48.25	
	ATOM		N C7									
	ATOM	1364	CA	THR			80.201	30.530	3.838		44.49	
	ATOM	1365	СВ	THR	А	∠40	81.413	29.633	4.106	1.00	45.53	А

	ATOM	1366	OG1	THR	Α	245	80.994	28.514	4.899	1.00	45.14 A
	ATOM	1367	CG2	THR	Α	245	82.486	30.403	4.873	1.00	42.13 A
	ATOM	1368	С	THR	Α	245	80.523	31.537	2.734	1.00	40.69 A
	ATOM	1369	0	THR			80.722	31.175	1.572		38.45 A
5	ATOM	1370		ALA			80.570	32.804	3.127		36.53 A
3			N								
	MOTA	1371	CA	ALA			80.816	33.915	2.219		34.68 A
	ATOM	1372	СВ	ALA	Α	246	81.106	35.186	3.023	1.00	34.13 A
	MOTA	1373	С	ALA	Α	246	81.896	33.718	1.164	1.00	33.21 A
	ATOM	1374	0	ALA	Α	246	81.655	33.958	-0.015	1.00	33.62 A
10	ATOM	1375	N	GLN			83.082	33.281	1.567		31.02 A
•	ATOM	1376	CA	GLN			84.151	33.112	0.595		31.05 A
	ATOM	1377	СВ	GLN			85.476	32.814	1.310		33.25 A
	MOTA	1378	CG	GLN			85.921	33.931	2.253		37.08 A
	ATOM	1379	CD	GLN	Α	247	87.378	33.831	2.665	1.00	40.56 A
15	ATOM	1380	OE1	GLN	Α	247	88.272	34.328	1.972	1.00	41.24 A
	ATOM	1381	NE2	GLN			87.626	33.180	3.794	1.00	41.86 A
	ATOM	1382	С	GLN			83.895	32.069	-0.488		28.53 A
							84.544				27.93 A
	ATOM	1383	0	GLN				32.093	-1.527		
	MOTA	1384	N	TYR			82.934	31.177	-0.267		28.01 A
20	ATOM	1385	CA	TYR	Α	248	82.643	30.115	-1.238	1.00	28.20 A
	ATOM	1386	CB	TYR	Α	248	82.725	28.757	-0.532	1.00	24.94 A
	ATOM	1387	CG	TYR	Α	248	84.064	28.533	0.126	1.00	23.77 A
	ATOM	1388	CD1	TYR			85.153	28.073	-0.611	1.00	23.01 A
	ATOM	1389	CE1				86.421	27.975	-0.039		24.66 A
25	ATOM	1390	CD2	TYR			84.270	28.879	1.464		24.01 A
23											
	ATOM	1391	CE2	TYR			85.535	28.785	2.050		24.49 A
	MOTA	1392	CZ	TYR			86.606	28.338	1.286		26.11 A
	ATOM	1393	OH	TYR			87.868	28.305	1.828		27.54 A
	ATOM	1394	С	TYR	Α	248	81.301	30.249	-1.961	1.00	28.78 A
30	ATOM	1395	0	TYR	Α	248	80.939	29.405	-2.777	1.00	30.26 A
	ATOM	1396	N	VAL	Α	249	80.576	31.319	-1.663	1.00	28.83 A
	ATOM	1397	CA	VAL	Α	249	79.281	31.584	-2.275	1.00	28.70 A
	ATOM	1398	СВ	VAL			78.625	32.803	-1.601		29.37 A
	ATOM	1399		VAL			77.333	33.163	-2.297		30.56 A
25											
35	ATOM	1400		VAL			78.376	32.488	-0.127		31.25 A
	MOTA	1401	С	VAL			79.404	31.837	-3.779		28.19 A
	ATOM	1402	0	VAL	Α	249	80.335	32.497	-4.231	1.00	27.69 A
	ATOM	1403	N	SER	Α	250	78.460	31.308	-4.549	1.00	28.16 A
	ATOM	1404	CA	SER	Α	250	78.476	31.481	-5.993	1.00	29.05 A
40	ATOM	1405	СВ	SER	Α	250	77.835	30.273	-6.691	1.00	31.08 A
	ATOM	1406	OG	SER			76.497	30.058	-6.264		31.33 A
		1407	C	SER			77.737	32.752	-6.376		29.69 A
	ATOM										
	ATOM	1408	0	SER			76.820	33.191	-5.685		29.14 A
	MOTA	1409	N			251	78.131	33.361	-7.494		29.35 A
45	ATOM	1410	CD	PRO	Α	251	79.147	32.917	-8.463	1.00	29.28 A
	ATOM	1411	CA	PRO	Α	251	77.477	34.592	-7.934	1.00	30.27 A
	ATOM	1412	CB	PRO	Α	251	78.214	34.932	-9.235	1.00	29.87 A
	ATOM	1413	CG	PRO	Α	251	78.687	33.588	-9.730	1.00	30.48 A
	ATOM	1414	С	PRO	Α	251	75.961	34.495	-8.114	1.00	30.86 A
50	ATOM	1415	0	PRO			75.246	35.442	-7.801		33.28 A
50		1416		GLU				33.367	-8.602		30.19 A
	ATOM		N				75.459				
	MOTA	1417	CA	GLU			74.014	33.244	-8.802		30.91 A
	ATOM	1418	СВ	GLU			73.649	31.903	-9.449		30.61 A
	MOTA	1419	CG	GLU			74.162	30.682	-8.689	1.00	33.88 A
55	ATOM	1420	CD	GLU	Α	252	75.493	30.171	-9.219	1.00	32.82 A
	ATOM	1421	OE1	GLU			76.277	30.987	-9.747	1.00	35.25 A
	ATOM	1422		GLU			75.756	28.956	-9.095		32.14 A
	ATOM	1423	C	GLU			73.260	33.390	-7.494		32.09 A
	ATOM	1424	0	GLU			72.157	33.928	-7.469		32.03 A
	AION	114 1	\supset	ОПО	А	272	12.101	JJ.J40	7.703	1.00	52.UI A

	ATOM	1425	N	LEU	Α	253	73.852	32.900	-6.408	1.00	33.87 A
	ATOM	1426	CA	LEU	Α	253	73.230	32.988	-5.096	1.00	35.16 A
	ATOM	1427	СВ	LEU	Α	253	74.031	32.183	-4.078	1.00	37.63 A
	ATOM	1428	CG	LEU	Δ	253	73.371	30.937	-3.479	1.00	40.98 A
5	ATOM	1429		LEU			74.302	30.321	-2.433		42.16 A
5				LEU			72.043				40.33 A
	ATOM	1430	CD2					31.314	-2.835		
	MOTA	1431	С	LEU			73.148	34.445	-4.640		37.20 A
	ATOM	1432	0	LEU			72.300	34.810	-3.820	1.00	37.33 A
	ATOM	1433	N	LEU	Α	254	74.036	35.276	-5.171	1.00	36.48 A
10	ATOM	1434	CA	LEU	Α	254	74.052	36.686	-4.816	1.00	37.76 A
	ATOM	1435	СВ	LEU	Α	254	75.481	37.235	-4.890	1.00	35.47 A
	ATOM	1436	CG	LEU			76.512	36.692	-3.899		32.31 A
	ATOM	1437		LEU			77.839	37.416	-4.108		32.18 A
	ATOM	1438		LEU			76.019	36.891	-2.474		29.68 A
15		1439	C	LEU			73.150	37.496	-5.737		39.82 A
13	ATOM										
	ATOM	1440	0	LEU			72.772	38.615	-5.409		39.15 A
	MOTA	1441	Ν	THR			72.805	36.919	-6.885		44.09 A
	ATOM	1442	CA	THR			71.959	37.594	-7.865		47.95 A
	ATOM	1443	СВ	THR	Α	255	72.591	37.544	-9.276	1.00	48.10 A
20	ATOM	1444	OG1	THR	Α	255	73.924	38.072	-9.227	1.00	48.96 A
	ATOM	1445	CG2	THR	Α	255	71.768	38.376	-10.253	1.00	50.10 A
	ATOM	1446	С	THR	А	255	70.538	37.032	-7.954	1.00	49.95 A
	ATOM	1447	0	THR			69.631	37.537	-7.300		51.66 A
	ATOM	1448	N	GLU			70.344	35.994	-8.764		52.84 A
25	ATOM	1449	CA	GLU			69.018	35.395	-8.939		55.77 A
23				GLU							55.24 A
	ATOM	1450	CB				69.036		-10.061		
	ATOM	1451	CG	GLU			70.360		-10.790		55.40 A
	MOTA	1452	CD	GLU			70.699		-11.681		55.34 A
	ATOM	1453	OE 1	GLU	Α	256	69.831		-12.480		55.36 A
30	ATOM	1454	OE2	GLU	Α	256	71.837	35.852	-11.593	0.00	55.36 A
	ATOM	1455	С	GLU	Α	256	68.451	34.743	-7.677	1.00	57.04 A
	ATOM	1456	0	GLU	Α	256	67.396	34.107	-7.732	1.00	56.82 A
	ATOM	1457	N	LYS	Α	257	69.137	34.911	-6.549	1.00	58.87 A
	ATOM	1458	CA	LYS			68.711	34.308	-5.286	1.00	60.38 A
35	ATOM	1459	СВ	LYS			67.607	35.151	-4.623	1.00	
00	ATOM	1460	CG	LYS			66.327	35.322	-5.430	0.00	
	ATOM	1461	CD	LYS			65.352	36.261	-4.731	0.00	
	ATOM	1462	CE	LYS			64.943	35.734	-3.363	0.00	
10	ATOM	1463	ΝZ	LYS			63.992	36.650	-2.674	0.00	
40	ATOM	1464	С	LYS			68.227	32.878	-5.546		61.40 A
	MOTA	1465	0	LYS			67.046	32.565	-5.389		61.84 A
	MOTA	1466	N	SER	Α	258	69.160	32.020		1.00	61.26 A
	MOTA	1467	CA	SER	Α	258	68.865	30.622	-6.271		61.31 A
	ATOM	1468	CB	SER	Α	258	68.105	30.548	-7.605	1.00	62.95 A
45	ATOM	1469	OG	SER	Α	258	68.707	31.374	-8.596	1.00	63.22 A
	MOTA	1470	С	SER	Α	258	70.149	29.771	-6.334	1.00	60.39 A
	ATOM	1471	0	SER			71.257	30.312	-6.329		60.58 A
	ATOM	1472	N	ALA			70.001	28.447	-6.393		57.62 A
	ATOM	1473	CA	ALA			71.159	27.551	-6.441		54.75 A
50		1474	CB	ALA			71.670	27.289	-5.025		54.90 A
50	ATOM										
	ATOM	1475	C	ALA			70.890	26.218	-7.147		52.13 A
	MOTA	1476	0	ALA			69.759	25.726	-7.175		51.63 A
	MOTA	1477	N	CYS			71.945	25.641	-7.712		48.49 A
	MOTA	1478	CA	CYS			71.848	24.371	-8.417		44.82 A
55	MOTA	1479	СВ	CYS	A	260	71.499	24.596	-9.890	1.00	46.78 A
	MOTA	1480	SG	CYS	Α	260	72.731	25.549	-10.821	1.00	53.48 A
	ATOM	1481	С	CYS	Α	260	73.176	23.643	-8.310	1.00	41.48 A
	ATOM	1482	0	CYS			74.085		-7.612		41.05 A
	ATOM	1483	N	LYS			73.288	22.525	-9.012		37.76 A
	111 011	1100	1.4		- 1		. 5 • 200	0_0	J. U.L.	1.00	5O A

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	ATOM	1484	CA	LYS			74.503	21.729	-8.980		34.90 A
	ATOM	1485	СВ	LYS	Α	261	74.394	20.587	-9.990	1.00	35.93 A
	ATOM	1486	CG	LYS	Α	261	73.239	19.644	-9.691	1.00	38.46 A
	ATOM	1487	CD	LYS			73.239		-10.601		39.70 A
_											
5	ATOM	1488	CE	LYS			72.117		-10.229	1.00	40.95 A
	ATOM	1489	NZ	LYS	Α	261	72.076	16.269	-11.110	1.00	41.64 A
	ATOM	1490	С	LYS	Α	261	75.751	22.556	-9.247	1.00	32.19 A
							76.780	22.366			30.08 A
	ATOM	1491	0	LYS					-8.595		
	ATOM	1492	N	SER	Α	262	75.651	23.480	-10.200	1.00	30.41 A
10	ATOM	1493	CA	SER	Α	262	76.771	24.337	-10.556	1.00	27.88 A
	ATOM	1494	СВ	SER	Z	262	76.361	25 333	-11.643	1 00	29.04 A
	ATOM	1495	OG	SER			76.398		-12.921		32.20 A
	MOTA	1496	С	SER	Α	262	77.325	25.095	-9.360	1.00	27.01 A
	ATOM	1497	0	SER	Α	262	78.515	25.403	-9.320	1.00	27.37 A
15	ATOM	1498	N	SER			76.469	25.406	-8.392		24.83 A
13											
	ATOM	1499	CA	SER			76.924	26.115	-7.201		26.29 A
	ATOM	1500	СВ	SER	Α	263	75.758	26.354	-6.242	1.00	26.59 A
	ATOM	1501	OG	SER	Α	263	74.830	27.254	-6.832	1.00	30.68 A
	ATOM	1502	С	SER			78.039	25.337	-6.506		25.15 A
20											
20	ATOM	1503	0	SER	Α	263	79.034	25.924	-6.078		25.38 A
	ATOM	1504	N	ASP	Α	264	77.884	24.019	-6.396	1.00	23.51 A
	ATOM	1505	CA	ASP	Ά	264	78.930	23.215	-5.773	1.00	22.06 A
	ATOM	1506	СВ	ASP			78.500	21.754	-5.613		23.87 A
	ATOM	1507	CG	ASP			77.378	21.577	-4.599		27.11 A
25	ATOM	1508	OD1	ASP	Α	264	77.276	22.402	-3.662	1.00	25.60 A
	ATOM	1509	OD2	ASP	Α	264	76.612	20.599	-4.730	1.00	26.16 A
	ATOM	1510	C	ASP			80.175	23.267	-6.642		20.62 A
	ATOM	1511	0	ASP	Α	264	81.289	23.339	-6.129	1.00	20.01 A
	ATOM	1512	N	LEU	Α	265	79.985	23.246	-7.959	1.00	18.87 A
30	ATOM	1513	CA	LEU	Α	265	81.113	23.275	-8.876	1.00	20.02 A
20	ATOM	1514	СВ	LEU			80.634		-10.322		19.94 A
	ATOM	1515	CG	LEU	Α	265	80.037	21.763	-10.672	1.00	21.08 A
	ATOM	1516	CD1	LEU	Α	265	79.580	21.771	-12.122	1.00	22.16 A
	ATOM	1517	CD2	LEU	Α	265	81.077	20,659	-10.449	1.00	16.76 A
35		1518	C	LEU			81.910	24.552	-8.705		20.53 A
33	ATOM										
	ATOM	1519	0	LEU	Α	265	83.130	24.563	-8.881		21.94 A
	ATOM	1520	N	TRP	Α	266	81.221	25.633	-8.361	1.00	21.74 A
	ATOM	1521	CA	TRP	Α	266	81.897	26.899	-8.138	1.00	20.89 A
	ATOM	1522	СВ	TRP			80.879	28.031	-7.960		22.97 A
40											
40	ATOM	1523	CG	TRP			81.477	29.309	-7.411		24.01 A
	MOTA	1524	CD2	TRP	Α	266	81.814	30.487	-8.152	1.00	23.31 A
	MOTA	1525	CE2	TRP	Α	266	82.391	31.404	-7.243	1.00	23.27 A
	ATOM	1526		TRP			81.689	30.858	-9.497		24.79 A
	ATOM	1527		TRP			81.850	29.555	-6.116		24.55 A
45	MOTA	1528	NE1	TRP	Α	266	82.401	30.811	-6.009	1.00	23.65 A
	MOTA	1529	CZ2	TRP	Α	266	82.839	32.663	-7.636	1.00	22.89 A
	ATOM	1530		TRP			82.139	32.116	-9.887		23.30 A
	ATOM	1531	CH2	TRP			82.705	33.000	-8.959		23.32 A
	ATOM	1532	С	TRP	Α	266	82.739	26.735	-6.877	1.00	20.30 A
50	MOTA	1533	0	TRP	Α	266	83.913	27.102	-6.853	1.00	20.60 A
	ATOM	1534	N	ALA			82.141	26.175	-5.832		18.06 A
	ATOM	1535	CA	ALA			82.868	25.966	-4.584		18.46 A
	ATOM	1536	СВ	ALA	Α	267	81.984	25.254	-3.561	1.00	17.96 A
	ATOM	1537	С	ALA			84.112	25.132	-4.877		18.05 A
55				ALA							
55	ATOM	1538	0				85.173	25.340	-4.287		17.35 A
	ATOM	1539	N	LEU			83.982	24.190	-5.799		17.12 A
	ATOM	1540	CA	LEU	Α	268	85.118	23.355	-6.157	1.00	18.45 A
	ATOM	1541	СВ	LEU			84.703	22.326	-7.204		17.67 A
	ATOM	1542	CG	LEU	А	200	85.809	21.436	-7.772	T.00	16.93 A

	ATOM	1543	CD1	LEU .	7\	268	86.333	20.495	-6.704	1 00	17.10 A
	ATOM	1544	CD2				85.258	20.493	-8.953		17.10 A
	ATOM	1545	С	LEU .			86.232	24.249	-6.705		19.64 A
-	ATOM	1546	0	LEU .			87.389	24.129	-6.306		18.99 A
5	MOTA	1547	N	GLY .			85.869	25.158	-7.606		19.16 A
	MOTA	1548	CA	GLY .			86.854	26.057	-8.178		18.25 A
	MOTA	1549	С	GLY .			87.604	26.804	-7.103		20.30 A
	ATOM	1550	0	GLY .			88.825	26.960	-7.178		20.24 A
	ATOM	1551	N	CYS .	A	270	86.874	27.266	-6.090	1.00	20.20 A
10	ATOM	1552	CA	CYS .	A	270	87.486	27.996	-4.986	1.00	20.73 A
	MOTA	1553	СВ	CYS .	Α	270	86.418	28.523	-4.031	1.00	21.05 A
	ATOM	1554	SG	CYS .	Α	270	85.292	29.703	-4.752	1.00	23.98 A
	ATOM	1555	С	CYS .	A	270	88.417	27.082	-4.206	1.00	20.77 A
	ATOM	1556	0	CYS .	Α	270	89.550	27.449	-3.878	1.00	22.00 A
15	ATOM	1557	N	ILE .			87.927	25.886	-3.907		19.32 A
	ATOM	1558	CA	ILE .			88.704	24.921	-3.147		18.46 A
	ATOM	1559	СВ	ILE .			87.872	23.668	-2.861		15.71 A
	ATOM	1560	CG2	ILE .			88.722	22.607	-2.182		16.51 A
	ATOM	1561	CG1				86.688	24.051	-1.974		14.97 A
20	ATOM	1562	CD1				85.785	22.891	-1.639		17.80 A
20	ATOM	1563	C	ILE .			90.001	24.546	-3.856		19.30 A
		1564	0	ILE .			91.062	24.532	-3.242		21.30 A
	ATOM						89.915				
	ATOM	1565	N	ILE .				24.253	-5.147		20.07 A
25	ATOM	1566	CA	ILE .			91.094	23.894	-5.906		21.50 A
25	ATOM	1567	CB	ILE .			90.758	23.693	-7.385		22.57 A
	ATOM	1568	CG2	ILE .			92.041	23.498	-8.184		21.91 A
	ATOM	1569	CG1	ILE .			89.818	22.495	-7.542		23.57 A
	ATOM	1570	CD1	ILE .			89.314	22.294	-8.949		24.20 A
	MOTA	1571	С	ILE .			92.112	25.010	-5.794		22.90 A
30	MOTA	1572	0	ILE .			93.287	24.783	-5.507		21.82 A
	MOTA	1573	N	TYR .			91.638	26.226	-6.028		24.81 A
	ATOM	1574	CA	TYR .	A	273	92.478	27.400	-5.969		25.15 A
	MOTA	1575	CB	TYR .	A	273	91.630	28.632	-6.255	1.00	26.04 A
	MOTA	1576	CG	TYR .	A	273	92.385	29.931	-6.173	1.00	27.80 A
35	MOTA	1577	CD1	TYR .	Α	273	92.715	30.500	-4.939	1.00	27.53 A
	ATOM	1578	CE1	TYR .	A	273	93.405	31.708	-4.870	1.00	27.30 A
	ATOM	1579	CD2	TYR .	A	273	92.765	30.602	-7.333	1.00	27.17 A
	ATOM	1580	CE2	TYR .	A	273	93.448	31.804	-7.277	1.00	26.68 A
	ATOM	1581	CZ	TYR .	Α	273	93.766	32.355	-6.050	1.00	28.05 A
40	ATOM	1582	OH	TYR .	Α	273	94.433	33.562	-6.018	1.00	30.80 A
	ATOM	1583	С	TYR .			93.139	27.521	-4.599	1.00	26.05 A
	ATOM	1584	0	TYR .			94.310	27.889	-4.489	1.00	24.45 A
	ATOM	1585	N	GLN .			92.380	27.205	-3.556		25.95 A
	ATOM	1586	CA	GLN .			92.896	27.299	-2.202		25.98 A
45	ATOM	1587	СВ	GLN .			91.743	27.209	-1.199		25.56 A
	ATOM	1588	CG	GLN .			92.169	27.422	0.233		25.42 A
	ATOM	1589	CD	GLN .			90.990	27.571	1.161		28.69 A
	ATOM	1590		GLN .			89.838	27.506	0.732		29.84 A
	ATOM	1591		GLN .			91.267	27.774	2.445		29.83 A
50		1592		GLN .							
30	ATOM		C				93.951	26.231	-1.915		25.08 A
	ATOM	1593	0	GLN .			94.862	26.452	-1.120		24.38 A
	ATOM	1594	N	LEU .			93.838	25.081	-2.567		24.42 A
	ATOM	1595	CA	LEU .			94.813	24.006	-2.369		25.43 A
	MOTA	1596	СВ	LEU .			94.335	22.713	-3.035		22.95 A
55	ATOM	1597	CG	LEU .			93.193	21.959	-2.354		25.67 A
	MOTA	1598		LEU .			92.817	20.702	-3.154		22.16 A
	MOTA	1599	CD2	LEU .	A	275	93.633	21.580	-0.950		23.32 A
	MOTA	1600	С	LEU .			96.171	24.376	-2.948	1.00	25.40 A
	ATOM	1601	0	LEU .	Α	275	97.212	24.071	-2.376	1.00	25.87 A

	MOTA	1602	N	VAL A	. 276	96.153	25.039	-4.094	1.00	25.78 A
	ATOM	1603	CA	VAL A	. 276	97.384	25.419	-4.759	1.00	26.12 A
	ATOM	1604	СВ	VAL A		97.170	25.522	-6.280		26.14 A
_	ATOM	1605		VAL A		98.492	25.783	-6.962		24.46 A
5	ATOM	1606	CG2	VAL A		96.531	24.248	-6.804		22.55 A
	ATOM	1607	С	VAL A	. 276	97.990	26.735	-4.275	1.00	27.83 A
	ATOM	1608	0	VAL A	. 276	99.210	26.849	-4.164	1.00	29.55 A
	ATOM	1609	N	ALA A	277	97.148	27.723	-3.990		26.88 A
		1610				97.639	29.023	-3.549		26.50 A
1.0	ATOM		CA	ALA A						
10	MOTA	1611	СВ	ALA A		96.765	30.126	-4.122		24.49 A
	ATOM	1612	С	ALA A	. 277	97.740	29.175	-2.035		26.79 A
	ATOM	1613	0	ALA A	. 277	98.465	30.042	-1.548	1.00	28.26 A
	ATOM	1614	N	GLY A	278	97.020	28.343	-1.290	1.00	26.17 A
	ATOM	1615	CA	GLY A		97.074	28.430	0.159		24.63 A
15		1616		GLY A			29.272	0.780		25.52 A
13	ATOM		C			95.971				
	ATOM	1617	0	GLY A		95.793	29.259	1.998		27.25 A
	MOTA	1618	N	LEU A	. 279	95.229	29.998	-0.051	1.00	24.94 A
	ATOM	1619	CA	LEU A	. 279	94.130	30.849	0.408	1.00	25.58 A
	ATOM	1620	СВ	LEU A	279	94.603	32.302	0.522	1.00	27.65 A
20	ATOM	1621	CG	LEU A		95.748	32.631	1.470		29.35 A
20						96.365	33.958			
	ATOM	1622		LEU A				1.075		30.47 A
	ATOM	1623	CD2	LEU A		95.232	32.671	2.892		29.70 A
	MOTA	1624	С	LEU A	. 279	92.987	30.822	-0.605	1.00	25.19 A
	ATOM	1625	0	LEU A	. 279	93.201	30.525	-1.781	1.00	25.34 A
25	ATOM	1626	N	PRO A		91.755	31.126	-0.165		23.60 A
	ATOM	1627	CD	PRO A		91.306	31.357	1.216		22.97 A
		1628		PRO A		90.628	31.133	-1.103		23.81 A
	ATOM		CA							
	MOTA	1629	СВ	PRO A		89.417	31.338	-0.195		25.19 A
	ATOM	1630	CG	PRO A	. 280	89.982	32.041	1.008	1.00	25.48 A
30	ATOM	1631	С	PRO A	. 280	90.855	32.295	-2.083	1.00	26.26 A
	ATOM	1632	0	PRO A	. 280	91.632	33.207	-1.792	1.00	25.42 A
	ATOM	1633	N	PRO A		90.178	32.284	-3.243		26.49 A
	ATOM	1634	CD	PRO A		89.182	31.285	-3.651		27.13 A
	ATOM	1635	CA	PRO A		90.307	33.316	-4.281		27.25 A
35	ATOM	1636	СВ	PRO A		89.522	32.727	-5.463		26.75 A
	MOTA	1637	CG	PRO A	. 281	89.354	31.291	-5.136	1.00	25.29 A
	ATOM	1638	С	PRO A	. 281	89.817	34.724	-3.954	1.00	27.30 A
	ATOM	1639	0	PRO A	281	90.497	35.709	-4.238	1.00	27.67 A
	ATOM	1640	N	PHE A		88.623	34.817	-3.388		27.79 A
40	ATOM	1641	CA	PHE A		88.034	36.107	-3.066		28.37 A
40										
	ATOM	1642	СВ	PHE A		86.563	36.086	-3.467		27.77 A
	ATOM	1643	CG	PHE A		86.335	35.557	-4.857		29.06 A
	MOTA	1644	CD1	PHE A	. 282	86.454	36.392	-5.965	1.00	28.74 A
	ATOM	1645	CD2	PHE A	. 282	86.077	34.207	-5.063	1.00	25.80 A
45	ATOM	1646	CE1	PHE A	282	86.324	35.887	-7.255	1.00	28.50 A
	ATOM	1647		PHE A		85.947	33.695	-6.346		26.04 A
						86.071				
	ATOM	1648	CZ	PHE A			34.535	-7.444		28.02 A
	MOTA	1649	С	PHE A		88.184	36.426	-1.589		29.95 A
	ATOM	1650	0	PHE A	. 282	87.600	35.763	-0.741		32.95 A
50	ATOM	1651	N	ARG A	. 283	88.977	37.445	-1.285	1.00	32.36 A
	ATOM	1652	CA	ARG A	. 283	89.215	37.843	0.100	1.00	33.06 A
	ATOM	1653	СВ	ARG A	283	90.622	37.432	0.520		33.69 A
	ATOM	1654	CG	ARG A		90.990	36.006	0.151		36.29 A
	ATOM	1655	CD	ARG A		92.341	35.635	0.727		38.81 A
55	ATOM	1656	NE	ARG A	. 283	93.415	36.423	0.133	1.00	41.73 A
	MOTA	1657	CZ	ARG A	. 283	93.783	36.338	-1.142	1.00	44.14 A
	ATOM	1658	NH1	ARG A		93.162	35.497	-1.958		45.19 A
	ATOM	1659		ARG A		94.772	37.094	-1.604		44.57 A
	ATOM	1660	С	ARG A	. 203	89.065	39.353	0.267	T.UU	32.44 A

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	MOTA	1661	0	ARG			89.429	40.118	-0.624		31.91 A
	MOTA	1662	N	ALA	Α	284	88.527	39.777	1.406	1.00	33.21 A
	ATOM	1663	CA	ALA	Α	284	88.348	41.199	1.682	1.00	32.82 A
	ATOM	1664	СВ	ALA			87.265	41.777	0.782		32.40 A
_											
5	ATOM	1665	С	ALA			88.004	41.445	3.147		32.98 A
	ATOM	1666	0	ALA	Α	284	87.779	40.502	3.913	1.00	32.53 A
	ATOM	1667	N	GLY	Α	285	87.961	42.723	3.520	1.00	32.60 A
											30.00 A
	ATOM	1668	CA	GLY			87.666	43.112	4.887		
	ATOM	1669	С	GLY	Α	285	86.355	42.637	5.486	1.00	29.37 A
10	ATOM	1670	0	GLY	Α	285	86.287	42.366	6.685	1.00	29.35 A
	ATOM	1671	N	ASN	Z	286	85.302	42.547	4.685	1 00	28.99 A
	ATOM	1672	CA	ASN			84.024	42.097	5.226		29.58 A
	ATOM	1673	CB	ASN	Α	286	83.238	43.281	5.801	1.00	29.54 A
	ATOM	1674	CG	ASN	Α	286	82.958	44.356	4.764	1.00	29.60 A
15	ATOM	1675		ASN			82.350	44.092	3.720		26.48 A
13											
	ATOM	1676	ND2	ASN			83.400	45.575	5.049		25.96 A
	MOTA	1677	С	ASN	Α	286	83.196	41.378	4.182	1.00	30.16 A
	ATOM	1678	0	ASN	Ά	286	83.551	41.357	3.004	1.00	31.70 A
	ATOM	1679	N	GLU			82.084	40.796	4.613		31.14 A
20											
20	MOTA	1680	CA	GLU			81.225	40.051	3.699		32.53 A
	MOTA	1681	СВ	GLU	Α	287	79.943	39.600	4.397	1.00	35.66 A
	ATOM	1682	CG	GLU	Α	287	80.168	38.813	5.666	1.00	43.05 A
							79.138	37.707			47.79 A
	ATOM	1683	CD	GLU					5.856		
	ATOM	1684	OE1	GLU	Α	287	77.933	37.959	5.616	1.00	49.01 A
25	MOTA	1685	OE2	GLU	Α	287	79.539	36.588	6.256	1.00	48.82 A
	ATOM	1686	С	GLU	Δ	287	80.853	40.837	2.457	1.00	30.19 A
	ATOM	1687	0	GLU			80.986	40.332	1.343		30.33 A
	MOTA	1688	N	TYR	Α	288	80.385	42.066	2.653	1.00	29.13 A
	MOTA	1689	CA	TYR	Α	288	79.972	42.922	1.541	1.00	27.98 A
30	ATOM	1690	СВ	TYR	Α	288	79.573	44.320	2.034	1.00	26.59 A
20	ATOM	1691	CG	TYR			79.080	45.217	0.917		26.43 A
	MOTA	1692	CD1	TYR	Α	288	77.799	45.060	0.385		28.06 A
	MOTA	1693	CE1	TYR	Α	288	77.350	45.854	-0.675	1.00	28.72 A
	ATOM	1694	CD2	TYR	Α	288	79.905	46.196	0.363	1.00	27.24 A
35	ATOM	1695	CE2	TYR			79.470	46.994	-0.697		28.55 A
33											
	ATOM	1696	CZ	TYR			78.192	46.814	-1.211		29.91 A
	MOTA	1697	OH	TYR	Α	288	77.765	47.571	-2.275	1.00	30.53 A
	ATOM	1698	С	TYR	Α	288	81.057	43.068	0.487	1.00	25.84 A
	ATOM	1699	0	TYR			80.790	42.940	-0.701		27.88 A
40											
40	ATOM	1700	N	LEU			82.279	43.344	0.919		24.24 A
	MOTA	1701	CA	LEU	Α	289	83.382	43.495	-0.018	1.00	26.60 A
	ATOM	1702	CB	LEU	Α	289	84.662	43.919	0.713	1.00	25.15 A
	ATOM	1703	CG	LEU			85.005	45.411	0.817		27.82 A
	ATOM	1704		LEU			83.830	46.277	0.354		27.32 A
45	ATOM	1705	CD2	LEU	Α	289	85.404	45.727	2.251	1.00	25.62 A
	ATOM	1706	С	LEU	Α	289	83.622	42.184	-0.736	1.00	27.45 A
	ATOM	1707	0	LEU			83.901	42.157	-1.933		30.18 A
	ATOM	1708	N	ILE			83.520	41.093	0.009		28.11 A
	MOTA	1709	CA	ILE	Α	290	83.726	39.770	-0.551	1.00	28.84 A
50	ATOM	1710	СВ	ILE	Α	290	83.565	38.710	0.545	1.00	29.67 A
	ATOM	1711		ILE			83.450	37.331	-0.071		31.47 A
	ATOM	1712		ILE			84.756	38.802	1.504		29.26 A
	ATOM	1713	CD1	ILE	Α	290	84.604	37.995	2.779	1.00	27.48 A
	ATOM	1714	С	ILE	Α	290	82.727	39.530	-1.676	1.00	27.99 A
55	ATOM	1715	0	ILE			83.090	39.110	-2.775		26.63 A
55											
	ATOM	1716	Ν	PHE			81.464	39.824	-1.406		28.54 A
	MOTA	1717	CA	PHE	Α	291	80.432	39.638	-2.407	1.00	27.14 A
	ATOM	1718	СВ	PHE			79.066	39.945	-1.807		28.37 A
	ATOM	1719	CG	PHE			78.674	39.024	-0.688		30.37 A
	ATOM	エィエフ	UG	ظللت	ч	- J I	10.0/4	JJ.U44	0.000	1.00	50.51 A

	ATOM	1720	CD1	PHE A	291	79.283	37.778	-0.543	1.00 30.07 A
	ATOM	1721	CD2	PHE A		77.658	39.377	0.194	1.00 30.07 A
	ATOM	1722		PHE A		78.885	36.897	0.463	1.00 23.74 A 1.00 32.11 A
	ATOM	1723		PHE A		77.253	38.502	1.202	1.00 32.11 A 1.00 32.76 A
-							37.259		1.00 32.76 A 1.00 32.01 A
5	ATOM	1724	CZ	PHE A		77.867		1.336	
	ATOM	1725	С	PHE A		80.690	40.525	-3.618	1.00 27.79 A
	ATOM	1726	0	PHE A		80.434	40.124	-4.755	1.00 26.52 A
	ATOM	1727	N	GLN A		81.200	41.730	-3.384	1.00 27.05 A
	ATOM	1728	CA	GLN A		81.478	42.613	-4.503	1.00 27.48 A
10	ATOM	1729	СВ	GLN A		82.072	43.945	-4.037	1.00 27.80 A
	ATOM	1730	CG	GLN A		81.041	44.984	-3.651	1.00 30.50 A
	ATOM	1731	CD	GLN A		81.630	46.381	-3.565	1.00 31.30 A
	MOTA	1732		GLN A		82.519	46.644	-2.762	1.00 33.17 A
	MOTA	1733	NE2	GLN A	. 292	81.133	47.284	-4.399	1.00 32.86 A
15	ATOM	1734	С	GLN A	. 292	82.442	41.934	-5.460	1.00 26.82 A
	ATOM	1735	0	GLN A	. 292	82.186	41.883	-6.664	1.00 28.03 A
	MOTA	1736	N	LYS A	. 293	83.539	41.402	-4.924	1.00 24.08 A
	ATOM	1737	CA	LYS A	. 293	84.542	40.739	-5.751	1.00 24.43 A
	ATOM	1738	СВ	LYS A	. 293	85.752	40.368	-4.901	1.00 26.19 A
20	ATOM	1739	CG	LYS A	. 293	86.456	41.580	-4.319	1.00 28.24 A
	ATOM	1740	CD	LYS A	. 293	87.750	41.213	-3.608	1.00 30.60 A
	ATOM	1741	CE	LYS A		88.555	42.468	-3.273	1.00 32.23 A
	ATOM	1742	NZ	LYS A		89.849	42.170	-2.591	1.00 32.86 A
	ATOM	1743	C	LYS A		84.008	39.500	-6.472	1.00 25.06 A
25	ATOM	1744	0	LYS A		84.350	39.236	-7.628	1.00 24.96 A
23	ATOM	1745	N	ILE A		83.163	38.740	-5.793	1.00 24.33 A
	ATOM	1746	CA	ILE A		82.593	37.552	-6.399	1.00 24.46 A
	ATOM	1747	CB	ILE A		81.725	36.800	-5.385	1.00 24.40 A 1.00 22.52 A
	ATOM	1748	CG2	ILE A		80.837	35.783	-6.093	1.00 22.32 A 1.00 23.14 A
30		1749	CG2	ILE A		82.632			1.00 23.14 A 1.00 21.54 A
30	ATOM						36.141	-4.345	1.00 21.34 A 1.00 19.38 A
	ATOM	1750	CD1	ILE A		81.892	35.535	-3.175	
	ATOM	1751	C	ILE A		81.761	37.885	-7.639	1.00 27.01 A
	ATOM	1752	0	ILE A		81.967	37.303	-8.704	1.00 23.93 A
25	ATOM	1753	N	ILE A		80.830	38.828	-7.513	1.00 29.79 A
35	ATOM	1754	CA	ILE A		79.983	39.168	-8.653	1.00 32.98 A
	ATOM	1755	СВ	ILE A		78.767	40.004	-8.228	1.00 33.96 A
	ATOM	1756	CG2	ILE A		77.980	39.246	-7.174	1.00 36.23 A
	ATOM	1757	CG1	ILE A		79.216	41.358	-7.682	1.00 35.79 A
	ATOM	1758	CD1			78.062	42.266	-7.300	1.00 37.79 A
40	ATOM	1759	С	ILE A		80.729	39.898	-9.757	1.00 33.17 A
	MOTA	1760	0	ILE A		80.212		-10.862	1.00 34.06 A
	ATOM	1761	N	LYS A		81.946	40.333	-9.462	1.00 33.65 A
	MOTA	1762	CA	LYS A		82.747		-10.468	1.00 34.81 A
	MOTA	1763	СВ	LYS A		83.353	42.293	-9.895	1.00 38.05 A
45	ATOM	1764	CG	LYS A		82.353	43.427	-9.714	1.00 40.12 A
	MOTA	1765	CD	LYS A	. 296	83.070	44.736	-9.401	1.00 44.01 A
	MOTA	1766	CE	LYS A	. 296	82.191	45.939	-9.731	1.00 46.66 A
	MOTA	1767	NZ	LYS A	. 296	82.972	47.209	-9.833	1.00 47.40 A
	MOTA	1768	С	LYS A	. 296	83.851	40.078	-10.945	1.00 34.15 A
50	ATOM	1769	0	LYS A	. 296	84.622	40.415	-11.847	1.00 33.48 A
	ATOM	1770	N	LEU A	. 297	83.907	38.897	-10.333	1.00 33.82 A
	MOTA	1771	CA	LEU A	. 297	84.904	37.890	-10.663	1.00 32.06 A
	ATOM	1772	СВ	LEU A	. 297	84.716		-12.110	1.00 32.43 A
	ATOM	1773	CG	LEU A		85.452		-12.538	1.00 33.09 A
55	ATOM	1774		LEU A		84.959		-11.697	1.00 31.88 A
	ATOM	1775		LEU A		85.206		-14.025	1.00 32.51 A
	ATOM	1776	C	LEU A		86.275		-10.476	1.00 32.23 A
	ATOM	1777	0	LEU A		87.180		-11.278	1.00 32.08 A
	ATOM	1778	N	GLU A		86.424	39.267	-9.395	1.00 33.56 A
	111 011	1.70		OHO M		J U • 12 1	22.201	J. J. J	1.00 00.00 A

	MOTA	1779	CA	GLU	Α	298	87.682	39.936	-9.110	1.00	35.66 A
	ATOM	1780	СВ	GLU	Α	298	87.405	41.274	-8.428	1.00	38.03 A
	ATOM	1781	CG	GLU			88.641	42.125	-8.236		42.97 A
_	MOTA	1782	CD	GLU			88.383	43.313	-7.338		46.19 A
5	MOTA	1783	OE 1	GLU			87.412	44.055	-7.602	1.00	48.41 A
	MOTA	1784	OE2	GLU	Α	298	89.153	43.504	-6.369	1.00	48.44 A
	ATOM	1785	С	GLU	Α	298	88.644	39.117	-8.245	1.00	34.35 A
	ATOM	1786	0	GLU			88.508	39.065	-7.021		35.64 A
	ATOM	1787	N	TYR			89.611	38.478	-8.894		32.46 A
10	ATOM	1788	CA	TYR	Α	299	90.624	37.678	-8.208	1.00	30.71 A
	ATOM	1789	СВ	TYR	Α	299	90.031	36.367	-7.672	1.00	26.01 A
	ATOM	1790	CG	TYR	Α	299	89.874	35.300	-8.730	1.00	26.77 A
	ATOM	1791		TYR			88.871	35.390	-9.699		26.60 A
		1792							-10.724		
1.7	ATOM			TYR			88.768				26.10 A
15	ATOM	1793	CD2	TYR			90.770	34.236	-8.807		22.56 A
	MOTA	1794	CE2	TYR	Α	299	90.677	33.291	-9.822	1.00	24.59 A
	ATOM	1795	CZ	TYR	Α	299	89.674	33.400	-10.781	1.00	26.34 A
	ATOM	1796	OH	TYR	Α	299	89.578	32.463	-11.791	1.00	22.44 A
		1797	C	TYR			91.720	37.374	-9.229		30.95 A
20	ATOM										
20	ATOM	1798	0	TYR			91.528		-10.425		28.80 A
	ATOM	1799	N	ASP	Α	300	92.865	36.891	-8.764	1.00	33.38 A
	ATOM	1800	CA	ASP	Α	300	93.954	36.582	-9.680	1.00	36.47 A
	ATOM	1801	СВ	ASP	Α	300	94.782	37.845	-9.931	1.00	42.34 A
	ATOM	1802	CG	ASP			95.014	38.644	-8.666		46.20 A
25	ATOM							38.085			49.27 A
25		1803		ASP			95.607		-7.719		
	ATOM	1804	OD2	ASP			94.599	39.826	-8.615		49.25 A
	MOTA	1805	С	ASP	Α	300	94.848	35.444	-9.188	1.00	35.61 A
	ATOM	1806	0	ASP	Α	300	94.857	35.113	-8.002	1.00	34.48 A
	ATOM	1807	N	PHE			95.602	34.854	-10.111	1.00	35.02 A
30	ATOM	1808	CA	PHE			96.477	33.737	-9.781		35.94 A
30											
	ATOM	1809	СВ	PHE			96.501		-10.909		34.28 A
	MOTA	1810	CG	PHE	Α	301	95.156	32.167	-11.301	1.00	32.40 A
	ATOM	1811	CD1	PHE	Α	301	94.358	32.856	-12.205	1.00	30.50 A
	ATOM	1812	CD2	PHE	Α	301	94.708	30.947	-10.803	1.00	31.83 A
35	ATOM	1813	CE1	PHE			93.131		-12.617		31.48 A
55	ATOM	1814	CE2	PHE			93.484		-11.206		31.37 A
	ATOM	1815	CZ	PHE			92.695		-12.114		31.44 A
	MOTA	1816	С	PHE	Α	301	97.916	34.134	-9.524	1.00	38.11 A
	ATOM	1817	0	PHE	Α	301	98.458	35.010	-10.196	1.00	39.06 A
40	ATOM	1818	N	PRO	Α	302	98.559	33.498	-8.535	1.00	40.47 A
	ATOM	1819	CD	PRO			98.053	32.554	-7.524		41.16 A
		1820	CA	PRO			99.955	33.843			41.88 A
	ATOM										
	ATOM	1821	СВ	PRO			100.248	33.131	-6.963		42.01 A
	ATOM	1822	CG	PRO	Α	302	99.328	31.947	-7.001	1.00	41.79 A
45	MOTA	1823	С	PRO	Α	302	100.721	33.265	-9.458	1.00	44.54 A
	ATOM	1824	0	PRO	Α	302	100.263	32.305	-10.082	1.00	44.30 A
	ATOM	1825	N	GLU			101.874		-9.770		47.35 A
	ATOM	1826	CA	GLU			102.667		-10.912		50.51 A
	ATOM	1827	СВ	GLU			103.859		-11.105		53.23 A
50	ATOM	1828	CG	GLU	Α	303	104.431	34.376	-12.520	1.00	56.85 A
	ATOM	1829	CD	GLU	Α	303	103.976	35.600	-13.314	1.00	59.62 A
	ATOM	1830	OE 1	GLU	Α	303	104.508	35.819	-14.424	1.00	60.43 A
		1831		GLU					-12.834		60.45 A
	ATOM						103.088				
	ATOM	1832	С	GLU			103.173		-10.829		50.70 A
55	ATOM	1833	0	GLU			103.692		-11.815		52.21 A
	ATOM	1834	N	ALA	Α	304	103.018	31.309	-9.672	1.00	49.61 A
	ATOM	1835	CA	ALA	Α	304	103.495	29.933		1.00	49.10 A
	$\Delta T \cap M$	1836	CB	ΔΤ.Δ	Δ	.50.4	104 077	29 774	-8 082	1 00	48 82 4
	ATOM ATOM	1836 1837	CB C	ALA ALA			104.077 102.422	29.779 28.869	-8.082 -9.713		48.82 A 47.90 A

	ATOM	1838	0	ALA	Α	304	102.703	27.666	-9.719	1.00	49.41 A
	ATOM	1839	N	PHE	Α	305	101.192	29.322	-9.899	1.00	44.69 A
	ATOM	1840	CA	PHE	Α	305	100.053	28.440	-10.089	1.00	40.05 A
	ATOM	1841	СВ	PHE	Α	305	98.809	29.301	-10.299	1.00	39.69 A
5	ATOM	1842	CG	PHE			97.568	28.729	-9.697		37.21 A
J	ATOM	1843					96.824		-10.379		35.36 A
	ATOM	1844	CD2	PHE			97.133	29.157	-8.445		37.52 A
	ATOM	1845	CE1	PHE			95.658	27.255	-9.825		34.59 A
	MOTA	1846		PHE			95.963	28.641	-7.880		37.01 A
10	ATOM	1847	CZ	PHE	Α	305	95.226	27.688	-8.575	1.00	35.13 A
	ATOM	1848	С	PHE	Α	305	100.197	27.435	-11.230	1.00	37.65 A
	ATOM	1849	0	PHE	Α	305	100.364	27.814	-12.389	1.00	36.24 A
	ATOM	1850	N	PHE	Α	306	100.120	26.150	-10.892	1.00	35.64 A
	ATOM	1851	CA	PHE			100.219		-11.884		32.40 A
15	ATOM	1852	CB	PHE			99.781		-11.268		29.92 A
13		1853	CG	PHE				23.456	-9.926		28.24 A
	ATOM						100.412				
	ATOM	1854	CD1	PHE			101.796	23.457	-9.770		27.43 A
	MOTA	1855		PHE			99.617	23.173	-8.816		28.59 A
	ATOM	1856		PHE			102.380	23.181	-8.526		29.55 A
20	ATOM	1857	CE2	PHE	Α	306	100.188	22.895	-7.566	1.00	29.06 A
	ATOM	1858	CZ	PHE	Α	306	101.575	22.901	-7.422	1.00	29.51 A
	ATOM	1859	С	PHE	Α	306	99.296	25.452	-13.047	1.00	32.76 A
	ATOM	1860	0	PHE			98.087	25.625	-12.861		34.51 A
	ATOM	1861	N	PRO			99.856		-14.262		31.43 A
25	ATOM	1862	CD	PRO			101.272		-14.569		30.74 A
23									-15.485		29.54 A
	ATOM	1863	CA	PRO			99.128				
	ATOM	1864	СВ	PRO			100.158		-16.579		29.48 A
	MOTA	1865	CG	PRO			101.437		-15.895		30.81 A
	MOTA	1866	С	PRO			97.826		-15.743		29.74 A
30	ATOM	1867	0	PRO	Α	307	96.795	25.804	-16.022	1.00	31.08 A
	ATOM	1868	N	LYS	Α	308	97.867	23.870	-15.660	1.00	28.47 A
	ATOM	1869	CA	LYS	Α	308	96.672	23.086	-15.904	1.00	27.92 A
	ATOM	1870	СВ	LYS	Α	308	97.044	21.619	-16.114	1.00	28.70 A
	ATOM	1871	CG	LYS			97.696		-17.460		30.04 A
35	ATOM	1872	CD	LYS			98.310		-17.595		33.76 A
	ATOM	1873	CE	LYS			99.106		-18.888		33.22 A
			NZ	LYS					-18.948		36.67 A
	ATOM	1874					99.897				
	ATOM	1875	С	LYS			95.632		-14.800		26.85 A
	ATOM	1876	0	LYS			94.433		-15.060		25.34 A
40	MOTA	1877	N	ALA			96.084		-13.574		24.70 A
	ATOM	1878	CA	ALA			95.145	23.685	-12.486	1.00	24.41 A
	MOTA	1879	СВ	ALA	Α	309	95.855	23.652	-11.146	1.00	22.65 A
	ATOM	1880	С	ALA	Α	309	94.523	25.051	-12.712	1.00	26.56 A
	ATOM	1881	0	ALA	Α	309	93.327	25.238	-12.493	1.00	28.91 A
45	ATOM	1882	N	ARG			95.335		-13.149	1.00	26.94 A
	ATOM	1883	CA	ARG			94.830		-13.402		27.56 A
	ATOM	1884	CB	ARG			95.961		-13.864		28.69 A
	ATOM	1885	CG	ARG			95.438		-14.480		31.42 A
50	ATOM	1886	CD	ARG			96.482		-14.634		33.72 A
50	MOTA	1887	NE	ARG			95.881		-15.233		37.73 A
	ATOM	1888	CZ	ARG			96.412		-15.198		38.44 A
	ATOM	1889	NH1	ARG	Α	310	97.572	33.297	-14.588	1.00	37.72 A
	ATOM	1890	NH2	ARG	Α	310	95.775	34.108	-15.767	1.00	37.74 A
	MOTA	1891	С	ARG	Α	310	93.743	27.280	-14.473	1.00	26.84 A
55	ATOM	1892	0	ARG			92.678		-14.344		26.39 A
	ATOM	1893	N	ASP			94.019		-15.527		26.91 A
	ATOM	1894	CA	ASP			93.069		-16.615		28.21 A
		1895	CB	ASP			93.682		-17.713		30.32 A
	ATOM										
	ATOM	1896	CG	ASP	А	311	92.850	∠5.494	-18.972	1.00	35.68 A

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	ATOM	1897		ASP			91.894		-19.040		38.27	
	ATOM	1898	OD2	ASP			93.145		-19.888		37.07	
	MOTA	1899	С	ASP			91.769	25.748	-16.108	1.00	27.22	Α
	MOTA	1900	0	ASP	Α	311	90.678	26.205	-16.449	1.00	29.64	Α
5	ATOM	1901	N	LEU	Α	312	91.886	24.715	-15.285	1.00	24.32	Α
	ATOM	1902	CA	LEU	Α	312	90.708	24.062	-14.728	1.00	23.48	Α
	ATOM	1903	СВ	LEU			91.118		-13.892		21.65	
	ATOM	1904	CG	LEU			90.067		-12.945		21.40	
	ATOM	1905		LEU			88.789		-13.694		16.90	
10	ATOM	1906		LEU			90.629		-12.294		19.67	
10				LEU							22.73	
	ATOM	1907	C				89.899		-13.871			
	ATOM	1908	0	LEU			88.684		-14.021		22.02	
	ATOM	1909	N	VAL			90.574		-12.972		22.12	
	ATOM	1910	CA	VAL			89.897		-12.108		21.16	
15	MOTA	1911	СВ	VAL	Α	313	90.893	27.440	-11.167	1.00	23.49	Α
	ATOM	1912	CG1	VAL	Α	313	90.221	28.679	-10.534	1.00	20.45	Α
	ATOM	1913	CG2	VAL	Α	313	91.369	26.487	-10.080	1.00	21.63	Α
	ATOM	1914	С	VAL	Α	313	89.161	27.771	-12.920	1.00	22.93	Α
	ATOM	1915	0	VAL	Α	313	88.051	28.168	-12.566	1.00	21.46	А
20	ATOM	1916	N	GLU			89.784		-14.001		23.15	
20	ATOM	1917	CA	GLU			89.156		-14.832		25.95	
	ATOM	1918	CB	GLU			90.127		-15.900		28.61	
	ATOM	1919	CG	GLU			91.319		-15.350		32.73	
2.5	ATOM	1920	CD	GLU			92.205		-16.453		35.94	
25	ATOM	1921		GLU			92.188		-17.554		40.67	
	ATOM	1922	OE2	GLU			92.923		-16.225		37.73	
	ATOM	1923	С	GLU	Α	314	87.891		-15.505		24.64	
	MOTA	1924	0	GLU	Α	314	87.030	29.528	-15.892	1.00	24.01	Α
	MOTA	1925	N	LYS	Α	315	87.775	27.428	-15.654	1.00	23.67	Α
30	ATOM	1926	CA	LYS	Α	315	86.588	26.874	-16.278	1.00	23.15	Α
	ATOM	1927	СВ	LYS	Α	315	86.937	25.594	-17.042	1.00	24.76	Α
	ATOM	1928	CG	LYS	Α	315	87.784		-18.299	1.00	22.90	Α
	ATOM	1929	CD	LYS	Α	315	88.223		-18.929		23.63	
	ATOM	1930	CE	LYS			89.079		-20.153		23.20	
35	ATOM	1931	NZ	LYS			88.332		-21.142		29.09	
55	ATOM	1932	C	LYS			85.509		-15.244		23.08	
		1933	0	LYS					-15.596		23.63	
	ATOM						84.386		-13.969			
	ATOM	1934	N	LEU			85.852				21.74	
10	ATOM	1935	CA	LEU			84.910		-12.876		21.89	
40	ATOM	1936	СВ	LEU			85.569		-11.760		20.54	
	ATOM	1937	CG	LEU			85.841		-12.090		20.69	
	ATOM	1938		LEU			86.600		-10.947		17.08	
	ATOM	1939	CD2	LEU	Α	316	84.514	23.558	-12.336		19.15	
	ATOM	1940	С	LEU	Α	316	84.404	27.860	-12.312	1.00	23.66	Α
45	ATOM	1941	0	LEU	Α	316	83.215	28.005	-12.013	1.00	25.40	Α
	ATOM	1942	N	LEU	Α	317	85.310	28.816	-12.149	1.00	24.48	Α
	ATOM	1943	CA	LEU			84.933	30.121	-11.637		25.52	
	ATOM	1944	СВ	LEU			86.123		-10.936		24.23	
	ATOM	1945	CG	LEU			86.656		-9.719		21.22	
50	ATOM	1946		LEU			87.718		-9.015		23.73	
50		1947		LEU					-8.773		21.36	
	ATOM						85.515					
	ATOM	1948	С	LEU			84.459		-12.815		26.00	
	ATOM	1949	0	LEU			85.148		-13.286		28.02	
	ATOM	1950	N	VAL			83.272		-13.293		27.50	
55	ATOM	1951	CA	VAL			82.643		-14.421		28.43	
	ATOM	1952	СВ	VAL			82.365		-15.558		28.13	
	ATOM	1953	CG1	VAL	Α	318	81.624	30.953	-16.694	1.00	29.20	Α
	ATOM	1954	CG2	VAL	Α	318	83.677	29.689	-16.045	1.00	27.12	Α
	ATOM	1955	С	VAL	Α	318	81.331	31.842	-13.896		29.21	

	ATOM	1956	0	VAL 2	A 3	318	80.559	31.120	-13.255	1.00	30.06 A
	ATOM	1957	N	LEU 2	A 3	319	81.082	33.121	-14.150	1.00	29.94 A
	ATOM	1958	CA	LEU 2	A 3	319	79.858	33.758	-13.671	1.00	30.57 A
	ATOM	1959	СВ	LEU 2	Δ :	319	79.808	35.214	-14.133	1.00	32.89 A
5	ATOM	1960	CG	LEU I			80.908		-13.553		35.26 A
J											
	ATOM	1961		LEU Z			80.741		-14.059		34.63 A
	MOTA	1962	CD2	LEU 2			80.835		-12.028		34.01 A
	ATOM	1963	С	LEU I			78.598		-14.117	1.00	30.01 A
	ATOM	1964	0	LEU 2	A 3	319	77.704	32.768	-13.316	1.00	30.48 A
10	ATOM	1965	N	ASP I	A 3	320	78.527	32.695	-15.397	1.00	30.13 A
	ATOM	1966	CA	ASP I	A 3	320	77.362	31.996	-15.919	1.00	29.97 A
	ATOM	1967	СВ	ASP 2	A 3	320	77.393	31.981	-17.444	1.00	32.99 A
	ATOM	1968	CG	ASP 2	Δ :	320	76.116		-18.040		36.86 A
	ATOM	1969		ASP I			75.495		-17.412		38.81 A
15		1970		ASP I			75.739		-19.142		38.26 A
13	ATOM										
	ATOM	1971	С	ASP I			77.373		-15.402		28.61 A
	MOTA	1972	0	ASP 2			78.244		-15.758		28.87 A
	ATOM	1973	N	ALA 2	A 3	321	76.398	30.233	-14.566		28.88 A
	ATOM	1974	CA	ALA 2	A 3	321	76.311	28.897	-13.980		28.04 A
20	MOTA	1975	CB	ALA 2	A 3	321	75.156	28.842	-12.990	1.00	25.11 A
	ATOM	1976	С	ALA 2	A 3	321	76.151	27.794	-15.021	1.00	27.83 A
	ATOM	1977	0	ALA Z	A 3	321	76.500	26.643	-14.773	1.00	27.26 A
	ATOM	1978	N	THR			75.632		-16.190		27.45 A
	ATOM	1979	CA	THR I			75.413		-17.243		27.18 A
25	ATOM	1980	CB	THR 2			74.294		-18.191		26.99 A
23											
	ATOM	1981	OG1	THR I			74.739		-18.940		27.15 A
	ATOM	1982	CG2	THR 2			73.045		-17.399		23.11 A
	MOTA	1983	С	THR I			76.654		-18.077		28.31 A
	ATOM	1984	0	THR 2	A 3	322	76.605	26.133	-19.027	1.00	28.80 A
30	ATOM	1985	N	LYS I	A 3	323	77.769	27.546	-17.727	1.00	28.30 A
	ATOM	1986	CA	LYS I	A 3	323	78.990	27.348	-18.491	1.00	28.51 A
	ATOM	1987	СВ	LYS 2	A 3	323	79.392	28.651	-19.172	1.00	30.27 A
	ATOM	1988	CG	LYS 2	Α 3	323	78.305	29.160	-20.095	1.00	35.72 A
	ATOM	1989	CD	LYS			78.839		-21.170		37.65 A
35	ATOM	1990	CE	LYS			77.722		-22.131		39.59 A
33	ATOM	1991	NZ	LYS I			77.088		-22.733		40.41 A
	ATOM	1992	С	LYS			80.154		-17.683		28.68 A
	ATOM	1993	0	LYS I			81.298		-18.119		29.54 A
	ATOM	1994	N	ARG .			79.866		-16.503		27.43 A
40	ATOM	1995	CA	ARG 2			80.921		-15.684		25.01 A
	ATOM	1996	CB	ARG 2	A 3	324	80.559	25.800	-14.205	1.00	22.81 A
	MOTA	1997	CG	ARG 2	A 3	324	80.489	27.223	-13.715	1.00	21.68 A
	ATOM	1998	CD	ARG 2	A 3	324	80.036	27.315	-12.277	1.00	20.65 A
	ATOM	1999	NE	ARG 2	A 3	324	79.655	28.689	-11.971	1.00	21.18 A
45	ATOM	2000	CZ	ARG 2			78.645	29.029	-11.180		19.20 A
	ATOM	2001		ARG 2			77.909		-10.598		19.05 A
	ATOM	2002		ARG 2			78.349		-11.004		19.45 A
	ATOM	2002	C	ARG I			81.161				24.64 A
									-16.073		
50	ATOM	2004	0	ARG 2			80.219		-16.290		23.78 A
50	MOTA	2005	N	LEU 2			82.433		-16.177		23.92 A
	ATOM	2006	CA	LEU 2			82.809		-16.526		25.53 A
	ATOM	2007	СВ	LEU 2	A 3	325	84.336	22.422	-16.558	1.00	25.18 A
	ATOM	2008	CG	LEU Z	A 3	325	84.995	21.178	-17.149	1.00	25.63 A
	ATOM	2009	CD1	LEU 2			84.541	20.949	-18.590	1.00	25.39 A
55	ATOM	2010		LEU Z			86.500		-17.087		23.10 A
	ATOM	2011	С	LEU Z			82.224		-15.466		25.01 A
	ATOM	2012	0	LEU I			82.449		-14.278		23.81 A
	ATOM	2013	N	GLY I			81.450		-15.900		26.41 A
			CA				80.850		-14.964		
	ATOM	2014	CA	GLY I	-1 J	J _ U	00.000	19.003	14.504	1.00	26.13 A

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	MOTA	2015	С	GLY			79.338		-14.835		29.31 A
	ATOM	2016	0	GLY			78.697		-14.444	1.00	31.67 A
	ATOM	2017	N	CYS	Α	327	78.753	20.918	-15.162	1.00	29.49 A
	ATOM	2018	CA	CYS	Α	327	77.308	21.073	-15.042	1.00	31.91 A
5	ATOM	2019	СВ	CYS			76.935		-14.982		31.78 A
5		2020		CYS							38.33 A
	ATOM		SG				77.084		-16.552		
	ATOM	2021	С	CYS			76.539		-16.175		32.76 A
	MOTA	2022	0	CYS	Α	327	77.096	20.069	-17.228	1.00	32.18 A
	ATOM	2023	N	GLU	Α	328	75.248	20.175	-15.952	1.00	33.60 A
10	ATOM	2024	CA	GLU	Α	328	74.400	19.497	-16.921		36.82 A
10	ATOM	2025	CB	GLU			72.951		-16.408		41.60 A
	ATOM	2026	CG	GLU			72.845		-14.863		48.96 A
	ATOM	2027	CD	GLU			72.000		-14.321		51.75 A
	ATOM	2028	OE1	GLU	Α	328	72.393	17.103	-14.509	1.00	52.77 A
15	ATOM	2029	OE2	GLU	Α	328	70.948	18.550	-13.696	1.00	52.29 A
	ATOM	2030	С	GLU			74.466		-18.317		35.83 A
	ATOM	2031	0	GLU			74.618		-19.318		34.85 A
	ATOM	2032	N	GLU			74.370		-18.378		33.75 A
	ATOM	2033	CA	GLU	Α	329	74.399	22.146	-19.650	1.00	32.37 A
20	ATOM	2034	СВ	GLU	Α	329	74.153	23.640	-19.439	1.00	34.70 A
	ATOM	2035	CG	GLU	Α	329	72.898	23.972	-18.640	1.00	38.53 A
	ATOM	2036	CD	GLU			73.017		-17.172		41.60 A
		2037							-16.548		44.03 A
	ATOM			GLU			74.048				
	ATOM	2038	OE2	GLU			72.080		-16.636		44.74 A
25	ATOM	2039	С	GLU	Α	329	75.711	21.947	-20.399	1.00	30.96 A
	ATOM	2040	0	GLU	Α	329	75.757	22.114	-21.617	1.00	28.90 A
	ATOM	2041	N	MET	Α	330	76.773	21.605	-19.673	1.00	29.20 A
	ATOM	2042	CA	MET			78.075		-20.291		27.90 A
		2043	CB	MET			79.190		-19.455		30.57 A
20	ATOM										
30	ATOM	2044	CG	MET			79.189		-19.446		32.33 A
	ATOM	2045	SD	MET	Α	330	79.488	24.269	-21.070	1.00	36.55 A
	ATOM	2046	CE	MET	Α	330	81.257	24.001	-21.239	1.00	35.61 A
	ATOM	2047	С	MET	Α	330	78.319	19.883	-20.443	1.00	27.32 A
	ATOM	2048	0	MET	Δ	330	79.452	19.436	-20.606	1.00	25.82 A
35	ATOM	2049	N	GLU			77.232		-20.365		25.18 A
33											
	ATOM	2050	CA	GLU			77.246		-20.526		24.56 A
	ATOM	2051	СВ	GLU			77.922		-21.848		23.55 A
	MOTA	2052	CG	GLU	Α	331	77.395	18.099	-23.030	1.00	25.42 A
	ATOM	2053	CD	GLU	Α	331	75.867	18.176	-23.082	1.00	28.50 A
40	ATOM	2054	OE1	GLU	Α	331	75.338	19.094	-23.750	1.00	31.00 A
	ATOM	2055	OE2	GLU	Δ	331	75.190		-22.467	1.00	30.18 A
	ATOM	2056	C	GLU			77.804		-19.396		24.55 A
	ATOM	2057	0	GLU			78.327		-19.629		25.02 A
	ATOM	2058	N	GLY			77.692		-18.172		22.83 A
45	ATOM	2059	CA	GLY	Α	332	78.098	16.564	-17.017	1.00	20.57 A
	ATOM	2060	С	GLY	Α	332	79.541	16.408	-16.606	1.00	20.81 A
	ATOM	2061	0	GLY	Α	332	80.430	17.167	-16.999	1.00	19.36 A
	ATOM	2062	N	TYR			79.753		-15.801		20.19 A
		2063		TYR							
50	ATOM		CA				81.053		-15.243		20.12 A
50	ATOM	2064	СВ	TYR			80.860		-14.052		20.05 A
	ATOM	2065	CG	TYR			80.483	14.902	-12.828	1.00	21.40 A
	ATOM	2066	CD1	TYR	Α	333	81.464	15.367	-11.956	1.00	22.85 A
	ATOM	2067	CE1	TYR	Α	333	81.141	16.181	-10.878	1.00	22.91 A
	ATOM	2068		TYR			79.160		-12.590		21.24 A
55											
55	ATOM	2069		TYR			78.827		-11.518		22.71 A
	ATOM	2070	CZ	TYR			79.827		-10.670		21.44 A
	ATOM	2071	OH	TYR			79.522		-9.621		24.72 A
	ATOM	2072	С	TYR	Α	333	82.076	14.484	-16.192	1.00	20.38 A
	ATOM	2073	0	TYR	Α	333	83.277	14.533	-15.910	1.00	18.82 A

	7.034	0074		GT	_	224	01 610	10 010	17 212	1 00	00 41	_
	MOTA	2074	N	GLY			81.610		-17.313		20.41	
	ATOM	2075	CA	GLY	A	334	82.534	13.378	-18.280	1.00	20.48	Α
	ATOM	2076	С	GLY	Α	334	83.611	14.367	-18.693	1.00	20.12	Α
	ATOM	2077	0	GLY	Α	334	84.808	14.105	-18.539	1.00	21.13	A
5	ATOM	2078	N	PRO			83.216		-19.230		19.75	
5		2079		PRO					-19.699		19.25	
	ATOM		CD				81.872					
	MOTA	2080	CA	PRO			84.218		-19.644		19.66	
	MOTA	2081	СВ	PRO	Α	335	83.366	17.644	-20.212	1.00	17.92	Α
	ATOM	2082	CG	PRO	Α	335	82.184	16.901	-20.784	1.00	19.24	Α
10	ATOM	2083	С	PRO	Α	335	85.115	16.967	-18.495	1.00	19.62	А
	ATOM	2084	0	PRO			86.315		-18.679		21.87	
	ATOM	2085	N	LEU			84.538		-17.307		19.91	
	MOTA	2086	CA	LEU			85.312		-16.147		19.06	
	ATOM	2087	СВ	LEU	Α	336	84.406	17.767	-14.914	1.00	18.05	Α
15	ATOM	2088	CG	LEU	Α	336	85.073	18.119	-13.571	1.00	18.25	Α
	ATOM	2089	CD1	LEU	Α	336	86.049	19.280	-13.746	1.00	15.57	А
	ATOM	2090		LEU			84.009		-12.538		15.31	
			C								17.85	
	ATOM	2091		LEU			86.424		-15.832			
	MOTA	2092	0	LEU			87.582		-15.690		17.14	
20	ATOM	2093	N	LYS	Α	337	86.075	15.317	-15.732	1.00	17.96	Α
	ATOM	2094	CA	LYS	Α	337	87.061	14.289	-15.438	1.00	19.15	Α
	ATOM	2095	СВ	LYS	Α	337	86.352	12.966	-15.134	1.00	21.53	Α
	ATOM	2096	CG	LYS			85.571		-13.821		25.58	
	ATOM	2097	CD	LYS			84.484		-13.715		26.69	
25												
25	ATOM	2098	CE	LYS			85.063		-13.571		29.78	
	MOTA	2099	NZ	LYS	A	337	83.979		-13.368		30.74	
	ATOM	2100	С	LYS	Α	337	88.065	14.120	-16.576	1.00	21.13	Α
	ATOM	2101	0	LYS	Α	337	89.170	13.631	-16.362	1.00	21.11	Α
	ATOM	2102	N	ALA	Α	338	87.697	14.549	-17.780	1.00	21.55	Α
30	ATOM	2103	CA	ALA			88.600		-18.922		22.23	
30		2103							-20.221			
	ATOM		СВ	ALA			87.802				21.66	
	ATOM	2105	С	ALA			89.604		-18.988		23.04	
	ATOM	2106	0	ALA	A	338	90.518		-19.800		22.63	
	MOTA	2107	N	HIS	Α	339	89.447	16.570	-18.131	1.00	23.26	Α
35	ATOM	2108	CA	HIS	Α	339	90.362	17.705	-18.148	1.00	23.33	A
	ATOM	2109	СВ	HIS	Α	339	90.017	18.680	-17.027	1.00	22.99	A
	ATOM	2110	CG	HIS			90.696		-17.156		23.43	
		2111		HIS			90.279		-17.710		24.32	
	ATOM											
4.0	MOTA	2112		HIS			91.993		-16.741		22.64	
40	ATOM	2113		HIS			92.346		-17.036		24.03	
	ATOM	2114	NE2	HIS	Α	339	91.324	22.056	-17.626	1.00	23.65	Α
	ATOM	2115	С	HIS	Α	339	91.833	17.302	-18.046	1.00	24.36	A
	ATOM	2116	0	HIS	Α	339	92.186	16.376	-17.317	1.00	24.27	Α
	ATOM	2117	N	PRO			92.713		-18.788		25.89	
45			CD									
43	ATOM	2118		PRO			92.394		-19.777		26.27	
	MOTA	2119	CA	PRO			94.151		-18.785		26.69	
	ATOM	2120	СВ	PRO	Α	340	94.727	18.861	-19.613	1.00	26.46	Α
	ATOM	2121	CG	PRO	Α	340	93.654	19.090	-20.636	1.00	25.56	Α
	ATOM	2122	С	PRO	Α	340	94.772	17.629	-17.396	1.00	27.13	Α
50	ATOM	2123	0	PRO			95.686		-17.167		28.89	
20	ATOM	2124	N	PHE			94.281		-16.466		26.76	
	ATOM	2125	CA	PHE			94.815		-15.110		25.83	
	ATOM	2126	СВ	PHE			94.100		-14.239		24.58	
	ATOM	2127	CG	PHE	Α	341	94.628	19.527	-12.835	1.00	23.75	Α
55	MOTA	2128	CD1	PHE	Α	341	95.890	20.060	-12.578	1.00	24.62	Α
	ATOM	2129		PHE			93.867		-11.765		24.82	
	ATOM	2130		PHE			96.386		-11.273		23.48	
	ATOM	2131		PHE			94.352		-10.454		23.61	
	ATOM	2132	CZ	PHE	А	341	95.614	тэ.673	-10.209	T.00	23.80	А

	ATOM	2133	С	PHE A	2/1	94.684	17.039 -14.458	1.00 25.53 A
	ATOM	2134	0	PHE A		95.453	16.698 -13.572	1.00 25.53 A
							16.248 -14.905	
	ATOM	2135	N	PHE A		93.718		1.00 26.56 A
-	ATOM	2136	CA	PHE A		93.486	14.928 -14.327	1.00 28.32 A
5	ATOM	2137	СВ	PHE A		91.992	14.724 -14.095	1.00 25.63 A
	ATOM	2138	CG	PHE A		91.374	15.731 -13.169	1.00 24.19 A
	ATOM	2139		PHE A		91.830	15.868 -11.859	1.00 24.72 A
	MOTA	2140	CD2			90.285	16.492 -13.579	1.00 21.46 A
	MOTA	2141		PHE A		91.200	16.744 -10.969	1.00 22.95 A
10	ATOM	2142	CE2			89.649	17.368 -12.699	1.00 19.82 A
	ATOM	2143	CZ	PHE A		90.105	17.491 -11.393	1.00 20.87 A
	ATOM	2144	С	PHE A		94.009	13.811 -15.217	1.00 31.08 A
	MOTA	2145	0	PHE A		93.655	12.643 -15.047	1.00 32.72 A
	MOTA	2146	N	GLU A	343	94.863	14.183 -16.159	1.00 33.50 A
15	ATOM	2147	CA	GLU A	343	95.446	13.250 -17.114	1.00 36.10 A
	ATOM	2148	СВ	GLU A	343	96.738	13.853 -17.676	1.00 38.76 A
	MOTA	2149	CG	GLU A	343	96.842	13.883 -19.194	1.00 44.39 A
	ATOM	2150	CD	GLU A	343	96.911	15.307 -19.750	1.00 48.43 A
	ATOM	2151	OE1	GLU A	343	97.665	16.143 -19.190	1.00 47.87 A
20	ATOM	2152	OE2	GLU A	343	96.217	15.587 -20.755	1.00 49.34 A
	ATOM	2153	С	GLU A	343	95.747	11.855 -16.552	1.00 35.54 A
	ATOM	2154	0	GLU A		95.210	10.847 -17.019	1.00 33.70 A
	ATOM	2155	N	SER A	344	96.604	11.810 -15.539	1.00 34.66 A
	ATOM	2156	CA	SER A		97.024	10.545 -14.950	1.00 33.91 A
25	ATOM	2157	СВ	SER A		98.421	10.712 -14.360	1.00 33.13 A
	ATOM	2158	OG	SER A		98.387	11.578 -13.242	1.00 30.32 A
	ATOM	2159	С	SER A		96.116	9.927 -13.886	1.00 33.50 A
	ATOM	2160	0	SER A		96.510	8.962 -13.234	1.00 32.98 A
	ATOM	2161	N	VAL A		94.908	10.448 -13.713	1.00 31.80 A
30	ATOM	2162	CA	VAL A		94.021	9.903 -12.689	1.00 31.70 A
50	ATOM	2163	CB	VAL A		93.039	10.981 -12.152	1.00 31.20 A
	ATOM	2164		VAL A		92.153	10.375 -11.079	1.00 29.96 A
	ATOM	2165	CG2			93.799	12.176 -11.601	1.00 27.23 A
	ATOM	2166	C	VAL A		93.175	8.707 -13.133	1.00 27.23 A
35	ATOM	2167	0	VAL A		92.597	8.712 -14.223	1.00 32.39 A
33	ATOM	2168	N	THR A		93.109	7.688 -12.279	1.00 32.33 A
	ATOM	2169	CA	THR A		92.285	6.511 -12.539	1.00 31.00 A
	ATOM	2170	CB	THR A		93.007	5.209 -12.149	1.00 32.94 A
	ATOM	2171		THR A		94.137	5.012 -13.013	1.00 33.81 A
40	ATOM	2172	CG2			92.060	4.022 -12.267	1.00 37.83 A
40	ATOM	2172	CGZ	THR A		91.051	6.700 -11.658	1.00 32.32 A 1.00 33.08 A
	ATOM	2173		THR A		91.031	6.460 -10.448	1.00 33.00 A
	ATOM	2174	O	TRP A		89.964	7.142 -12.274	1.00 34.21 A
		2176	N CA	TRP A		88.741	7.427 -11.549	1.00 31.78 A
45	ATOM ATOM		CB					
43		2177		TRP A		87.769	8.171 -12.463	1.00 28.28 A
	MOTA	2178	CG	TRP A		88.303	9.476 -12.937	1.00 23.66 A
	ATOM	2179		TRP A		88.263	10.722 -12.231	1.00 23.03 A
	ATOM	2180		TRP A		88.927	11.678 -13.031	1.00 20.77 A
50	ATOM	2181		TRP A		87.731	11.121 -10.999	1.00 20.57 A
50	ATOM	2182		TRP A		88.969	9.718 -14.102	1.00 21.92 A
	ATOM	2183		TRP A		89.348	11.041 -14.168	1.00 22.23 A
	MOTA	2184		TRP A		89.074	13.008 -12.640	1.00 21.04 A
	ATOM	2185		TRP A		87.876	12.444 -10.611	1.00 20.11 A
	ATOM	2186		TRP A		88.544	13.372 -11.430	1.00 20.44 A
55	MOTA	2187	С	TRP A		88.014	6.267 -10.899	1.00 34.19 A
	MOTA	2188	0	TRP A		87.382	6.440 -9.854	1.00 34.97 A
	MOTA	2189	N	GLU A		88.108	5.089 -11.502	1.00 35.77 A
	MOTA	2190	CA	GLU A		87.405	3.913 -11.000	1.00 36.41 A
	MOTA	2191	СВ	GLU A	348	87.600	2.740 -11.977	1.00 36.95 A

	ATOM	2192	CG	GLU	Α	348	88.990	2.626	-12.588	0.00	36.86 A
	ATOM	2193	CD	GLU	Α	348	89.173	3.510	-13.812	0.00	36.91 A
	ATOM	2194	OE 1	GLU			89.119	4 750	-13.677		36.92 A
_	ATOM	2195	OE2	GLU			89.370		-14.916		36.92 A
5	ATOM	2196	С	GLU	Α	348	87.668	3.435	-9.563	1.00	36.38 A
	ATOM	2197	0	GLU	Α	348	86.773	2.866	-8.935	1.00	38.29 A
	ATOM	2198	N	ASN	Α	349	88.857	3.669	-9.019	1.00	34.41 A
	ATOM	2199	CA	ASN			89.134	3.182	-7.668		33.02 A
	MOTA	2200	СВ	ASN			89.848	1.844	-7.765		34.07 A
10	ATOM	2201	CG	ASN	Α	349	91.220	1.978	-8.381	1.00	35.48 A
	ATOM	2202	OD1	ASN	Α	349	91.409	2.742	-9.324	1.00	35.13 A
	ATOM	2203	ND2	ASN	Α	349	92.188	1.235	-7.852	1.00	38.04 A
	ATOM	2204	С	ASN			89.970	4.116	-6.804		30.73 A
	MOTA	2205	0	ASN			90.878	3.672	-6.106		30.66 A
15	ATOM	2206	Ν	LEU	Α	350	89.662	5.403	-6.850	1.00	28.42 A
	ATOM	2207	CA	LEU	Α	350	90.390	6.397	-6.072	1.00	27.13 A
	MOTA	2208	СВ	LEU	Α	350	89.655	7.737	-6.128	1.00	25.19 A
	ATOM	2209	CG	LEU			89.803	8.543	-7.418		25.97 A
	MOTA	2210		LEU			88.841	9.732	-7.428		26.30 A
20	ATOM	2211	CD2	LEU	Α	350	91.242	9.014	-7.521	1.00	27.40 A
	ATOM	2212	С	LEU	Α	350	90.581	5.999	-4.614	1.00	26.30 A
	ATOM	2213	0	LEU	Α	350	91.645	6.201	-4.036	1.00	26.73 A
	ATOM	2214	N	HIS			89.547	5.424	-4.024		27.16 A
	MOTA	2215	CA	HIS			89.593	5.044	-2.622		28.60 A
25	ATOM	2216	CB	HIS	Α	351	88.184	4.748	-2.124	1.00	29.94 A
	ATOM	2217	CG	HIS	Α	351	88.111	4.503	-0.653	1.00	30.99 A
	ATOM	2218	CD2	HIS	Α	351	88.324	5.329	0.399	1.00	31.86 A
	ATOM	2219		HIS			87.790	3.275	-0.118		29.43 A
• •	ATOM	2220		HIS			87.804	3.356	1.202		31.81 A
30	ATOM	2221	NE2	HIS			88.125	4.592	1.541	1.00	32.90 A
	ATOM	2222	С	HIS	Α	351	90.509	3.873	-2.298	1.00	28.99 A
	ATOM	2223	0	HIS	Α	351	90.875	3.677	-1.141	1.00	28.53 A
	ATOM	2224	N	GLN			90.865	3.088	-3.307		30.57 A
2.5	ATOM	2225	CA	GLN			91.764	1.959	-3.095		33.42 A
35	ATOM	2226	СВ	GLN	Α	352	91.563	0.880	-4.162		35.01 A
	ATOM	2227	CG	GLN	Α	352	90.696	-0.289	-3.737	1.00	37.07 A
	ATOM	2228	CD	GLN	Α	352	89.275	0.123	-3.474	1.00	39.83 A
	ATOM	2229	OE 1	GLN			88.676	0.856	-4.267		41.90 A
		2230	NE2	GLN				-0.351	-2.365		39.86 A
40	ATOM						88.712				
40	MOTA	2231	С	GLN			93.197	2.457	-3.173		33.85 A
	ATOM	2232	0	GLN	Α	352	94.126	1.782	-2.734		35.32 A
	ATOM	2233	N	GLN	Α	353	93.368	3.647	-3.734	1.00	32.53 A
	ATOM	2234	CA	GLN	Α	353	94.693	4.216	-3.886	1.00	32.78 A
	ATOM	2235	СВ	GLN			94.666	5.298			32.07 A
15											
45	ATOM	2236	CG	GLN			94.373	4.739	-6.345		31.94 A
	ATOM	2237	CD	GLN	Α	353	94.206	5.819	-7.382	1.00	32.50 A
	ATOM	2238	OE 1	GLN	Α	353	95.008	6.749	-7.452	1.00	35.33 A
	MOTA	2239	NE2	GLN	Α	353	93.167	5.701	-8.204	1.00	31.02 A
	ATOM	2240	C	GLN			95.246	4.779	-2.588		33.27 A
50											
50	ATOM	2241	0	GLN			94.494	5.209	-1.717		32.38 A
	MOTA	2242	N	THR	Α	354	96.570	4.746	-2.462	1.00	33.29 A
	ATOM	2243	CA	THR	Α	354	97.239	5.267	-1.280	1.00	34.35 A
	ATOM	2244	СВ	THR	Α	354	98.615	4.601	-1.069		35.88 A
	ATOM	2245		THR			98.430	3.232	-0.690		36.70 A
55											
55	ATOM	2246		THR			99.403	5.325	0.027		36.08 A
	MOTA	2247	С	THR	Α	354	97.440	6.760	-1.478		33.06 A
	MOTA	2248	0	THR	Α	354	98.120	7.181	-2.403	1.00	31.33 A
	ATOM	2249	N	PRO	Α	355	96.844	7.581	-0.604		33.40 A
	ATOM	2250	CD	PRO			96.000	7.220	0.544		31.90 A
	711 01.1	2200	01	1110	1.7	333	50.000	, . 220	0.544	1.00	51.50 A

	ATOM	2251	CA	PRO	Α	355	96.974	9.035	-0.710	1.00	34.90	А
	ATOM	2252	СВ	PRO	Α	355	96.156	9.543	0.475	1.00	33.68	Α
	ATOM	2253	CG	PRO	Α	355	95.160	8.452	0.698	1.00	33.37	Α
	ATOM	2254	С	PRO	Α	355	98.428	9.475	-0.623	1.00	36.27	Α
5	ATOM	2255	0	PRO	A	355	99.196	8.960	0.191	1.00	35.70	Α
	ATOM	2256	N	PRO	Α	356	98.824	10.433	-1.464	1.00	37.66	Α
	ATOM	2257	CD	PRO	Α	356	98.010	11.198	-2.423		38.22	
	ATOM	2258	CA	PRO			100.205	10.916	-1.441		39.93	
	ATOM	2259	СВ	PRO			100.227	11.944	-2.570		38.83	
10	ATOM	2260	CG	PRO			98.818	12.466	-2.580		38.26	
	ATOM	2261	С			356	100.532	11.534	-0.085		41.87	
	ATOM	2262	0	PRO			99.696	12.209	0.506		40.91	
	ATOM	2263	N	ALA			101.741	11.286	0.409		46.23	
	ATOM	2264	CA	ALA			102.160	11.837	1.691		51.16	
15	ATOM	2265	СВ	ALA			103.587	11.410	2.001		49.78	
15	ATOM	2266	C	ALA			102.077	13.354	1.589		54.64	
	ATOM	2267	0	ALA			102.591	13.942	0.637		55.14	
	ATOM	2268	N	LEU			101.419	13.985	2.559		58.59	
	ATOM	2269	CA	LEU			101.276	15.437	2.552		62.92	
20	ATOM	2270	CB	LEU			100.107	15.866	3.441		62.51	
20	ATOM	2271	CG	LEU			98.732	15.752	2.783		63.05	
	ATOM	2272		LEU			97.657	16.251	3.737		63.34	
	ATOM	2272		LEU			98.721	16.570	1.494		62.56	
	ATOM	2274	CDZ	LEU			102.536	16.173	2.984		65.81	
25	ATOM	2275	0	LEU			102.536	16.559	4.148		66.45	
23	ATOM	2276	N	THR			103.441	16.368	2.025	1.00		
	ATOM	2277	CA	THR			104.715	17.057	2.236		72.25	
	ATOM	2278	CB	THR			104.719	18.594	2.271		73.17	
	ATOM	2279		THR			103.564	18.937	3.284		75.38	
30	ATOM	2279		THR			104.030	19.101	0.916		72.93	
30	ATOM	2281	C	THR			105.468	16.627	3.497		73.76	
	ATOM	2282	0	THR			105.400	15.683	4.180		74.61	
	ATOM	2283		THR			106.523	17.237	3.780		75.50	
	ATOM	2284	OH2	TIP		1	82.965	32.402	-3.946		13.32	
35	ATOM	2285	OH2	TIP	S	2	91.556		-17.557		22.11	
33	ATOM	2286	OH2	TIP		3	87.391	33.155	-1.722		22.84	
	ATOM	2287	OH2		S	4	69.033	3.499	13.879		22.91	
	ATOM	2288	OH2		S	5	81.088		-18.406		24.13	
	ATOM	2289		TIP		6	75.641	16.130	8.209		26.44	
40	ATOM	2290		TIP		7	74.760	20.961	3.347		27.74	
4 0	ATOM	2291		TIP		8	75.152	6.784	5.545		22.53	
	ATOM	2292		TIP		9	77.282		-17.666		35.96	
	ATOM	2293		TIP		10	81.785	8.968	-8.072		25.44	
	ATOM	2294		TIP		11	78.609	24.424	-2.074		22.05	
45	ATOM	2295		TIP		12	94.883	8.256	-9.981		37.17	
73	ATOM	2296		TIP		13	73.164	38.970	-1.072		35.95	
		2297		TIP		14	78.806	27.556	-3.116		39.27	
	ATOM			TIP		15	89.050	8.041	10.604		23.40	
	ATOM	2298 2299		TIP		16	73.265		-3.301		26.94	
50	ATOM ATOM	2300		TIP		18	84.081	40.376 33.371	4.243		30.61	
50		2300		TIP		19	78.571	-0.530	16.531		26.61	
	ATOM							3.703				
	ATOM	2302		TIP TIP		21	70.088 79.212		17.559		28.94	
	ATOM	2303		TIP		22			-18.791 -16.153		26.94	
55	ATOM	2304				23	91.672		-16.153		30.26	
55	ATOM	2305		TIP		25	104.173		-7.204		31.65	
	ATOM	2306		TIP		27	87.578		-20.604		25.98	
	MOTA	2307		TIP		28	82.272		-16.021		27.40	
	ATOM	2308		TIP		29	100.496	13.074	-9.812		37.92	
	MOTA	2309	OH2	TIP	Ŋ	30	65.147	10.515	28.440	1.00	40.03	S

	MOTA	2310	OH2	TIP	S	31	90.721	38.800	-4.631	1.00	42.09	S
	ATOM	2311	OH2	TIP	S	32	83.367	23.841	15.654	1.00	36.15	S
	ATOM	2312	он2	TIP	g	33	87.754	11.897	23.760	1 00	26.76	q
_	ATOM	2313		TIP	S	34	77.755	13.485	-15.395		31.85	
5	ATOM	2314	OH2	TIP	S	35	79.767	43.115	5.371		35.26	
	MOTA	2315	OH2	TIP	S	37	80.173	32.998	6.198	1.00	40.03	S
	ATOM	2316	OH2	TIP	S	40	85.958	19.110	24.502	1.00	24.42	S
	ATOM	2317			S	42	77.719	-0.391	23.732		39.71	
											35.43	
10	ATOM	2318			S	44	92.563	36.428	-5.574			
10	ATOM	2319	OH2	TIP	S	45	90.942	34.092	3.570	1.00	43.64	S
	MOTA	2320	OH2	TIP	S	46	74.357	32.157	-13.849	1.00	33.31	S
	ATOM	2321	OH2	TIP	S	47	90.220	14.449	16.172	1.00	34.34	S
	ATOM	2322		TIP	S	48	77.876		-13.863	1 00	23.53	q
				TIP		50	76.289				37.74	
1.5	ATOM	2323			S				-11.572			
15	ATOM	2324	OH2	TIP	S	51	76.619	2.787	-2.969		35.95	
	ATOM	2325	OH2	TIP	S	52	65.118	19.629	24.370	1.00	34.85	S
	ATOM	2326	OH2	TIP	S	53	99.690	31.473	-13.046	1.00	48.21	S
	ATOM	2327	ОН2	TIP	g	54	88.376	36.865	3.454		38.54	
20	ATOM	2328		TIP		57	91.236	10.819	18.279		40.76	
20	ATOM	2329	OH2	TIP	S	59	100.017		-14.622		41.65	
	ATOM	2330	OH2	TIP	S	63	87.188	25.521	11.438	1.00	41.53	S
	ATOM	2331	OH2	TIP	S	65	90.264	19.625	12.286	1.00	24.22	S
	ATOM	2332	OH2	TIP	S	66	83.805	26.254	-18.365	1.00	37.50	S
	ATOM	2333	OH2	TIP	S	68	78.394	7.378	2.855		23.47	
25												
25	ATOM	2334	OH2		S	74	85.541		-18.436		37.35	
	ATOM	2335	OH2	TIP	S	76	98.981	8.707	2.808	1.00	47.34	S
	MOTA	2336	OH2	TIP	S	78	87.802	19.118	22.522	1.00	39.99	S
	ATOM	2337	OH2	TIP	S	80	92.438	3.105	2.517	1.00	37.27	S
	ATOM	2338		TIP		81	75.580	-0.821	22.186		36.41	
20												
30	ATOM	2339	OH2		S	82	60.506	24.278	21.938		31.55	S
	ATOM	2340	OH2	TIP	S	83	92.298		-21.183		42.32	
	ATOM	2341	OH2	TIP	S	84	74.351	4.211	-3.464	1.00	32.53	S
	ATOM	2342	OH2	TIP	S	85	76.502	25.963	-21.839	1.00	41.89	S
	ATOM	2343	ОН2	TIP	S	86	97.965	13.142	9.216		41.76	
35	ATOM	2344	OH2	TIP	S	87	78.657	4.418	3.361			S
33												
	ATOM	2345	OH2		S	88	93.633	28.572	3.429		34.30	
	MOTA	2346	OH2	TIP	S	89	104.691	20.306	-7.235	1.00	32.75	S
	MOTA	2347	OH2	TIP	S	91	98.360	16.754	-15.558	1.00	37.92	S
	ATOM	2348	OH2	TIP	S	92	88.175	32.723	-14.088	1.00	38.91	S
40	ATOM	2349	ОН2		S	93	96.974		-17.613		34.47	
10		2350		TIP			85.585	22.346	15.199		41.12	
	ATOM					94						
	ATOM	2351		TIP			80.948		7.892		12.04	
	MOTA	2352	OH2	TIP	S	101	76.653	29.202	-3.527	1.00	22.10	S
	MOTA	2353	OH2	TIP	S	102	74.980	8.979	-7.975	1.00	21.17	S
45	ATOM	2354	OH2	TIP	S	103	88.843	28.393	3.994	1.00	30.94	S
	ATOM	2355		TIP			76.862	8.067			20.20	
	ATOM	2356		TIP			66.435	30.702	8.817		35.87	
	ATOM	2357		TIP			67.384	7.757	8.860		39.38	
	ATOM	2358	OH2	TIP	S	110	66.852	4.666	22.301	1.00	32.75	S
50	ATOM	2359	OH2	TIP	S	111	72.391	2.229	-3.501	1.00	51.07	S
	ATOM	2360		TIP				7.061	-7.886		35.49	
	ATOM	2361		TIP			74.466		-12.357		45.36	
	ATOM	2362	OH2	TIP	S	122	79.225	28.627			30.68	
	ATOM	2363	OH2	TIP	S	124	59.090	22.126	22.498	1.00	35.94	S
55	ATOM	2364	OH2	TIP	S	126	73.715		-13.973		44.35	
	ATOM	2365		TIP			105.619		-11.256		43.80	
	ATOM	2366		TIP					-16.090		39.40	
	ATOM	2367		TIP					-10.875		45.74	
	ATOM	2368	OH2	TIP	S	136	77.820	12.663	6.090	1.00	47.18	S

	ATOM	2369	OH2	TIP	S	142	90.942	35.947	-13.582	1.00	48.16	S
	ATOM	2370	OH2	TIP		146	67.351	6.830	24.075		36.66	
			OH2				98.067	12.182	-7.216		38.66	
	ATOM	2371		TIP		148						
-	ATOM	2372				156	75.211		-20.582		45.56	
5	ATOM	2373	OH2	TIP	S	158	72.261	20.575	12.175			S
	ATOM	2374	OH2	TIP	S	166	77.289	42.685	7.086		42.23	
	MOTA	2375	OH2	TIP	S	174	65.330	6.552	20.003	1.00	42.22	S
	ATOM	2376	OH2	TIP	S	176	88.027	20.872	-20.665	1.00	35.09	S
	ATOM	2377	OH2	TIP	S	178	99.488	29.517	-16.497	1.00	44.21	S
10	ATOM	2378	OH2	TIP	S	182	93.851	13.830	-20.448	1.00	50.19	S
	ATOM	2379	OH2	TIP		192	83.811	26.388	9.460		39.52	
	ATOM	2380		TIP		193	91.704	42.080	2.405		40.67	
				GLC								
	ATOM	2381				1	82.624	0.887	12.473		47.94	
	ATOM	2382		GLC		1	82.240	2.160	13.000		48.49	
15	MOTA	2383		GLC		1	83.237	3.235	12.553		46.87	
	ATOM	2384	014	GLC	G	1	84.544	2.903	13.022	1.00	46.62	G
	ATOM	2385	C15	GLC	G	1	82.817	4.591	13.117	1.00	45.80	G
	ATOM	2386	016	GLC	G	1	83.746	5.589	12.703	1.00	43.50	G
	ATOM	2387	012	GLC	G	5	86.722	-2.593	0.107	1.00	39.62	G
20	ATOM	2388		GLC		5	86.245	-1.364	-0.429		44.37	
20	ATOM	2389		GLC		5	86.764	-0.193	0.394		44.36	
						5	86.355				47.64	
	ATOM	2390		GLC				-0.326	1.761			
	ATOM	2391		GLC		5	86.231	1.132	-0.195		45.11	
	ATOM	2392		GLC		5	86.666	1.310	-1.557		42.61	
25	ATOM	2393	012	GLC	G	8	87.512	4.414	-5.278	1.00	38.37	G
	MOTA	2394	C11	GLC	G	8	86.362	5.220	-5.023	1.00	34.16	G
	ATOM	2395	C13	GLC	G	8	85.750	5.654	-6.351	1.00	35.54	G
	ATOM	2396	014	GLC	G	8	86.717	6.392	-7.111	1.00	37.03	G
	ATOM	2397		GLC		8	84.521	6.523	-6.082		35.46	
30	ATOM	2398		GLC		8	83.948	6.931	-7.319		33.79	
50	ATOM	2399		STO		1	82.178	19.404	9.614		23.98	
	ATOM	2400	033	STO		1	83.091	19.645	10.691		24.40	
	ATOM	2401	C25	STO		1	82.557	20.621	11.610		19.84	
	ATOM	2402		STO		1	83.748	21.455	12.055		20.35	
35	ATOM	2403	N31	STO	$_{\rm L}$	1	84.251	22.242	10.916	1.00	22.56	$_{\rm L}$
	MOTA	2404	C32	STO	$_{\rm L}$	1	83.716	23.544	10.481	1.00	20.91	$_{\rm L}$
	ATOM	2405	C27	STO	$_{\rm L}$	1	84.847	20.523	12.559	1.00	19.37	$_{\rm L}$
	ATOM	2406	C28	STO	L	1	84.278	19.595	13.658	1.00	18.70	L
	ATOM	2407	029	STO	L	1	82.889	19.845	13.980	1.00	20.08	L
40	ATOM	2408	C24	STO		1	81.939	19.930	12.872		21.85	
.0	ATOM	2409	C35	STO		1	80.791	20.824	13.403		20.12	
	ATOM	2410	N6	STO			81.456	18.689	12.528		19.30	
						1						
	ATOM	2411	C5	STO		1	80.172	18.450	12.023		16.04	
	ATOM	2412	C4	STO		1	79.039	19.219	11.690		14.17	
45	ATOM	2413	С3	STO		1	77.901	18.569	11.148		14.32	
	ATOM	2414	C2	STO	$_{\rm L}$	1	77.899	17.158	10.946	1.00	14.05	$_{ m L}$
	ATOM	2415	C1	STO	L	1	79.035	16.386	11.282	1.00	13.54	L
	ATOM	2416	C23	STO	L	1	80.154	17.053	11.812	1.00	16.42	L
	ATOM	2417	C22	STO	L	1	81.361	16.522	12.164		17.74	
50	ATOM	2418	С7	STO		1	82.162	17.525	12.606		18.84	
20	ATOM	2419	C8	STO		1	83.501	17.279	12.972		18.69	
	ATOM	2420	N9	STO		1	84.462	18.150	13.376		19.59	
	ATOM	2421		STO		1	85.663	17.477	13.561		19.11	
	ATOM	2422		STO		1	86.968	17.838	13.942		16.81	
55	ATOM	2423		STO		1	87.961	16.831	14.007		20.66	
	ATOM	2424	C13	STO	L	1	87.645	15.476	13.689	1.00	20.30	L
	ATOM	2425	C14	STO	L	1	86.329	15.117	13.306	1.00	19.66	\mathbf{L}
	ATOM	2426		STO		1	85.364	16.127	13.248		18.74	
	ATOM	2427		STO		1	84.049	16.022	12.899		19.21	
		·			_	_				_,,,,		

	MOTA	2428		STO		1	83.217	14.936		1.00 18.26 L
	MOTA	2429	C21			1	81.934	15.217		1.00 17.21 L
	MOTA	2430	C20	STO		1	81.325	14.098		1.00 17.68 L
	MOTA	2431	N19	STO		1	82.281	13.080		1.00 13.64 L
5	MOTA	2432	C18	STO		1	83.457	13.603		1.00 16.89 L
	MOTA	2433	030	STO		1	84.493	12.981		1.00 15.41 L
	MOTA	2434	S	SO4	Ι	1	64.914	7.877	16.247	1.00 82.11 I
	MOTA	2435	01	SO4	Ι	1	63.624	8.415	15.778	1.00 82.68 I
	MOTA	2436	02	SO4		1	65.841	8.992		1.00 82.73 I
10	MOTA	2437	03	SO4	Ι	1	65.479	7.010		1.00 83.33 I
	MOTA	2438	04	SO4	Ι	1	64.709	7.088		1.00 82.04 I
	ATOM	2439	S	SO4	Ι	2	68.379	-7.029		1.00112.82 I
	MOTA	2440	01	SO4	Ι	2	66.992	-6.526		1.00112.60 I
	ATOM	2441	02	SO4	Ι	2	68.850	-7.226		1.00112.21 I
15	ATOM	2442	03	SO4	Ι	2	68.426	-8.312		1.00112.24 I
	ATOM	2443	04	SO4	I	2	69.249	-6.051		1.00112.72 I
	ATOM	2444	S	SO4	Ι	3	84.927	-1.874	12.302	1.00 79.99 I
	MOTA	2445	01	SO4	Ι	3	84.408	-1.334	13.568	1.00 79.90 I
	ATOM	2446	02	SO4	Ι	3	84.442	-1.050		1.00 80.43 I
20	ATOM	2447	03	SO4	Ι	3	84.453	-3.263		1.00 79.92 I
	ATOM	2448	04	SO4	Ι	3	86.402	-1.845		1.00 80.52 I
	ATOM	2449	S	SO4	Ι	4	80.577	9.632		1.00 98.23 I
	MOTA	2450	01	SO4	Ι	4	79.725	9.060	28.972	1.00 96.88 I
	MOTA	2451	02	SO4	Ι	4	82.000	9.461	29.683	1.00 97.80 I
25	MOTA	2452	03	SO4	Ι	4	80.304	8.944	31.309	1.00 98.08 I
	MOTA	2453	04	SO4	I	4	80.281	11.069	30.178	1.00 98.08 I
	MOTA	2454	S	SO4	Ι	5	89.310	6.131	25.915	1.00110.86 I
	MOTA	2455	01	SO4	I	5	89.025	6.456	27.331	1.00110.48 I
	MOTA	2456	02	SO4	Ι	5	88.042	6.095	25.151	1.00110.12 I
30	MOTA	2457	03	SO4	I	5	89.970	4.810	25.844	1.00110.72 I
	MOTA	2458	04	SO4	I	5	90.205	7.155		1.00110.02 I
	MOTA	2459	02	PO4	Ρ	100	64.527	26.252		1.00 88.98 P
	ATOM	2460	03	PO4	Ρ	100	66.482	25.155		1.00 88.39 P
	MOTA	2461	04	PO4	Ρ	100	66.688	26.504	3.376	1.00 87.87 P
35	ATOM	2462	01	PO4	Ρ	100	66.264	27.565		1.00 88.80 P
	ATOM	2463	P	PO4	Ρ	100	65.992	26.368		1.00 88.61 P
	ATOM	2464	СВ	LEU		145	73.932	8.398		0.50 21.29 AC2
	ATOM	2465	CG	LEU		145	72.901	8.606		0.50 21.65 AC2
	MOTA	2466		LEU		145	71.904	9.671		0.50 21.60 AC2
40	MOTA	2467		LEU		145	72.195			0.50 19.61 AC2
	MOTA	2468	СВ	ASN		214	88.968	8.625		0.50 22.34 AC2
	MOTA	2469	CG	ASN		214	89.705	8.084		0.50 22.01 AC2
	MOTA	2470		ASN		214	89.240	7.153		0.50 22.82 AC2
	MOTA	2471	ND2	ASN		214	90.859	8.660		0.50 22.69 AC2
45	MOTA	2472	СВ	ASP		216	93.187	5.546		0.50 25.98 AC2
	MOTA	2473	CG	ASP		216	91.789	5.828		0.50 27.09 AC2
	MOTA	2474		ASP		216	91.587	6.896		0.50 28.49 AC2
	MOTA	2475	OD2	ASP		216	90.896	4.982	5.110	0.50 28.20 AC2
	END									

Example 8: Co-ordinates for PDK1 fragment co-crystallised with UCN-

01

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.50 A
    REMARK starting r= 0.1919 free r= 0.2582
                    r= 0.1894 free r= 0.2567
    REMARK final
    REMARK B rmsd for bonded mainchain atoms= 1.412 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.205 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.401 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.256 target= 2.5
    REMARK rweight= 0.1000 (with wa= 3.1611)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.387 b= 123.387 c= 47.115 alpha= 90 beta=
    90 gamma= 120
    REMARK parameter file 1 : /ddl/david/refinement/MY CNS/prot.par
    REMARK parameter file 2 : /dd1/david/refinement/MY_CNS/ucn01.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
    REMARK parameter file 5
    /dd1/david/refinement/MY_CNS/glycerol.par
    REMARK molecular structure file: ../generate/generate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../data/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.50
    REMARK initial B-factor correction applied to fobs :
    REMARK B11= -4.722 B22= -4.722 B33=
REMARK B12= -3.572 B13= 0.000 B23=
                                                 9.444
                                                 0.000
    REMARK B-factor correction applied to coordinate array B:
    REMARK bulk solvent: density level= 0.3837 e/A^3, B-factor=
    40.9071 A^2
    REMARK reflections with |Fobs|/sigma F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range: 14485 (
35
   100.0 %)
    REMARK number of unobserved reflections (no entry or |F|=0):
            0.7 %)
    101 (
    REMARK number of reflections rejected:
                                                         0 (
                                                               0.0 %)
    REMARK total number of reflections used:
                                                         14384 ( 99.3 % )
    REMARK number of reflections in working set: 13795 ( 95.2 % )
    REMARK number of reflections in test set:
                                                         589 ( 4.1 % )
                                47.115 90.00 90.00 120.00 P 32 2 1
    CRYST1 123.387 123.387
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE:25-Mar-2003 17:21:21
                                               created by user: david
   REMARK VERSION:1.0
    MOTA
              1 CB ALA A 73
                                     67.051 -3.293 12.591 1.00 59.77 A
               2 C ALA A 73
                                     67.941 -4.753 14.416 1.00 61.14 A
    MOTA
               3 O ALA A 73
                                     67.184 -5.270 15.240 1.00 61.61 A
    MOTA
    ATOM
               4 N ALA A 73
                                     66.523 -5.729 12.643 1.00 58.89 A
    ATOM
              5 CA ALA A 73
                                     67.564 -4.697 12.943 1.00 60.69 A
               6 N PRO A 74
                                     69.130 -4.241 14.770 1.00 61.63 A
    ATOM
                                  70.264 -3.830 13.918 1.00 61.72 A 69.514 -4.278 16.187 1.00 61.34 A 70.918 -3.663 16.181 1.00 61.79 A 71.458 -4.072 14.818 1.00 61.47 A 68.523 -3.481 17.047 1.00 60.16 A 67.625 -2.817 16.519 1.00 60.77 A
    MOTA
              7 CD PRO A 74
                                     70.264 -3.830 13.918 1.00 61.72 A
              8 CA PRO A 74
    ATOM
              9 CB PRO A 74
    ATOM
             10 CG PRO A 74
55
    ATOM
             11 C PRO A 74
    ATOM
             12 O PRO A 74
    ATOM
```

	ATOM	13	N	ALA A	75	68.680	-3.562	18.368	1.00 58	3.13 A
	ATOM	14	CA	ALA A	75	67.815	-2.828	19.292	1.00 54	1.74 A
	ATOM	15	СВ	ALA A	75	68.048	-3.309	20.731	1.00 54	
	ATOM	16	С	ALA A	75	68.175	-1.349	19.177	1.00 51	
5	ATOM	17	0	ALA A	75	69.313	-1.005	18.851	1.00 52	2.46 A
	ATOM	18	N	LYS A	76	67.215	-0.473	19.427	1.00 46	5.96 A
	ATOM	19	CA	LYS A	76	67.507	0.947	19.354	1.00 43	
	ATOM	20	СВ	LYS A	76	66.270	1.756	19.744	1.00 42	2.81 A
	ATOM	21	CG	LYS A	76	66.177	3.116	19.087	1.00 41	L.81 A
10	ATOM	22	CD	LYS A	76	65.926	2.983	17.590	1.00 40).56 A
	ATOM	23	CE	LYS A	76	65.691	4.343	16.943	1.00 42	
	ATOM	24	NZ	LYS A	76	65.362	4.231	15.495	1.00 42	
	ATOM	25	С	LYS A	76	68.639	1.218	20.351	1.00 41	L.25 A
	ATOM	26	0	LYS A	76	68.599	0.741	21.488	1.00 41	L.68 A
15	ATOM	27	N	LYS A	77	69.655	1.960	19.936	1.00 37	
13										
	ATOM	28	CA	LYS A	77	70.748	2.255	20.849	1.00 35	
	ATOM	29	СВ	LYS A	77	72.016	2.619	20.074	1.00 34	1.13 A
	ATOM	30	CG	LYS A	77	72.427	1.570	19.053	1.00 32	2.68 A
	ATOM	31	CD	LYS A	77	73.927	1.537	18.858	1.00 33	
20										
20	ATOM	32	CE	LYS A	77	74.366	0.471	17.849	1.00 31	
	ATOM	33	NZ	LYS A	77	73.796	-0.863	18.164	1.00 34	1.76 A
	ATOM	34	С	LYS A	77	70.313	3.408	21.743	1.00 34	1.79 A
	ATOM	35	0	LYS A	77	69.319	4.077	21.458	1.00 34	4 2 N A
					78					
	ATOM	36	N	ARG A		71.023	3.626	22.845	1.00 34	
25	ATOM	37	CA	ARG A	78	70.687	4.723	23.759	1.00 34	
	ATOM	38	CB	ARG A	78	69.694	4.247	24.839	1.00 38	3.43 A
	ATOM	39	CG	ARG A	78	70.027	2.884	25.353	1.00 42	2.71 A
	ATOM	40	CD	ARG A	78	69.355	2.424	26.625	1.00 48	
	ATOM	41	NE	ARG A	78	70.365	1.702	27.412	1.00 56	
30	ATOM	42	CZ	ARG A	78	70.428	0.355	27.518	1.00 57	7.88 A
	ATOM	43	NH1	ARG A	78	69.519	-0.397	26.838	1.00 58	3.45 A
	ATOM	44		ARG A	78	71.335	-0.195	28.369	1.00 59	
	ATOM	45	С	ARG A	78	71.967	5.330	24.382	1.00 32	
	MOTA	46	0	ARG A	78	73.066	4.777	24.278	1.00 31	L.42 A
35	ATOM	47	N	PRO A	79	71.844	6.509	24.997	1.00 30	0.46 A
	ATOM	48	CD	PRO A	79	70.616	7.284	25.232	1.00 28	3.96 A
						72.997				
	ATOM	49	CA	PRO A	79		7.172	25.609		0.38 A
	ATOM	50	СВ	PRO A	79	72.350	8.303	26.405	1.00 28	
	ATOM	51	CG	PRO A	79	71.169	8.642	25.568	1.00 27	1.83 A
40	ATOM	52	С	PRO A	79	73.889	6.287	26.468	1.00 29	9.47 A
	ATOM	53	0	PRO A	79	75.108	6.377	26.391	1.00 29	
	ATOM	54	N	GLU A	80	73.268	5.435	27.279	1.00 29	
	ATOM	55	CA	GLU A	80	73.975	4.533	28.179	1.00 29	∂.55 A
	ATOM	56	CB	GLU A	80	72.980	3.768	29.043	1.00 32	2.88 A
45	ATOM	57	CG	GLU A	80	71.996	4.643	29.798	1.00 40	1.36 A
15										
	ATOM	58	CD	GLU A	80	71.014	5.367	28.879	1.00 44	
	ATOM	59	OE1	GLU A	80	70.422	4.700	28.000	1.00 46	5.94 A
	ATOM	60	OE2	GLU A	80	70.828	6.598	29.038	1.00 45	5.47 A
	ATOM	61	С	GLU A	80	74.872	3.524	27.479	1.00 28	3.32 A
50	ATOM	62	0	GLU A	80	75.709	2.894	28.126	1.00 28	
50										
	ATOM	63	N	ASP A	81	74.698	3.342	26.168	1.00 26	
	ATOM	64	CA	ASP A	81	75.528	2.384	25.441	1.00 23	3.59 A
	ATOM	65	СВ	ASP A	81	74.834	1.888	24.184	1.00 25	5.08 A
	ATOM	66	CG	ASP A	81	73.510	1.225	24.477	1.00 28	
55										
55	ATOM	67		ASP A	81	73.369	0.625	25.578	1.00 29	
	ATOM	68	OD2	ASP A	81	72.617	1.294	23.601	1.00 28	3.33 A
	ATOM	69	С	ASP A	81	76.856	2.967	25.046	1.00 23	3.24 A
	ATOM	70	0	ASP A	81	77.716	2.257	24.519	1.00 24	
		71	N		82					
	ATOM	/ <u>T</u>	IA	PHE A	04	77.036	4.259	25.309	1.00 21	L. 34 A

	ATOM	72	CA	PHE	A	82	78.272	4.930	24.946	1.00	20.86 A
	ATOM	73	СВ	PHE	Α	82	77.992	6.029	23.929	1.00	18.34 A
	ATOM	74	CG	PHE	Α	82	77.355	5.536	22.683	1.00	19.18 A
	ATOM	75		PHE		82	78.138	5.099	21.610		19.28 A
5	ATOM	76		PHE		82	75.974	5.462	22.588		17.82 A
)											
	ATOM	77	CE1	PHE		82	77.551	4.597	20.461		17.94 A
	ATOM	78	CE2	PHE	A	82	75.371	4.961	21.449	1.00	19.08 A
	ATOM	79	CZ	PHE	Α	82	76.164	4.525	20.376	1.00	20.45 A
	ATOM	80	С	PHE	Α	82	78.982	5.555	26.105	1.00	21.71 A
10	ATOM	81	0	PHE	Α	82	78.418	5.739	27.173	1.00	24.82 A
	ATOM	82	N	LYS		83	80.244	5.865	25.869		21.83 A
	ATOM	83	CA	LYS		83	81.077	6.555	26.823		22.27 A
	ATOM	84	СВ	LYS		83	82.327	5.750	27.148		24.03 A
	ATOM	85	CG	LYS	A	83	83.074	6.320	28.340		30.99 A
15	ATOM	86	CD	LYS	Α	83	84.465	6.827	27.993	1.00	35.16 A
	ATOM	87	CE	LYS	Α	83	85.465	5.683	27.945	1.00	39.06 A
	ATOM	88	ΝZ	LYS	Α	83	85.512	4.974	29.266	1.00	41.00 A
	ATOM	89	C	LYS		83	81.462	7.775	25.998		22.51 A
20	ATOM	90	0	LYS		83	82.324	7.677	25.120		23.24 A
20	ATOM	91	N	PHE		84	80.800	8.907	26.227		20.27 A
	ATOM	92	CA	PHE	Α	8 4	81.118	10.098	25.454	1.00	19.31 A
	ATOM	93	СВ	PHE	Α	8 4	80.016	11.145	25.605	1.00	19.95 A
	ATOM	94	CG	PHE	Α	84	78.683	10.694	25.075	1.00	20.81 A
	ATOM	95	CD1	PHE	А	84	77.855	9.879	25.835	1.00	21.62 A
25	ATOM	96	CD2	PHE		84	78.278	11.035	23.804		20.47 A
	ATOM	97	CE1	PHE		8 4	76.665	9.418	25.339		19.26 A
	ATOM	98		PHE		84	77.073	10.568	23.300		18.97 A
	ATOM	99	CZ	PHE		84	76.276	9.764	24.068		19.78 A
			C			84	82.463	10.680	25.863		19.58 A
20	ATOM	100		PHE							
30	ATOM	101	0	PHE		84	82.888	10.540	26.998		20.60 A
	ATOM	102	N	GLY		85	83.141	11.307	24.913		19.33 A
	ATOM	103	CA	GLY		85	84.434	11.909	25.169		18.23 A
	ATOM	104	С	GLY		85	84.480	13.368	24.743	1.00	19.96 A
	ATOM	105	0	GLY	A	85	83.533	14.124	24.962	1.00	20.02 A
35	ATOM	106	N	LYS	A	86	85.568	13.764	24.101	1.00	20.79 A
	ATOM	107	CA	LYS	A	86	85.736	15.159	23.704	1.00	22.45 A
	ATOM	108	СВ	LYS	A	86	87.168	15.400	23.210	1.00	22.06 A
	ATOM	109	CG	LYS		86	87.399	15.048	21.751		23.37 A
	ATOM	110	CD	LYS		86	88.832	14.591	21.505		26.45 A
40											30.25 A
40	ATOM	111	CE	LYS		86	89.451	15.275	20.294		
	ATOM	112	NZ	LYS		86	89.771	16.721	20.553		33.08 A
	ATOM	113	С	LYS		86	84.750	15.668	22.661		21.50 A
	ATOM	114	0	LYS	Α	86	84.154	14.900	21.916		21.98 A
	ATOM	115	N	ILE	Α	87	84.582	16.985	22.647	1.00	20.15 A
45	ATOM	116	CA	ILE	Α	87	83.712	17.661	21.705	1.00	19.38 A
	ATOM	117	СВ	ILE	A	87	83.270	19.037	22.272	1.00	17.37 A
	ATOM	118	CG2	ILE		87	82.724	19.935	21.163		15.07 A
	ATOM	119		ILE		87	82.222	18.800	23.371		18.62 A
	ATOM	120		ILE		87	81.848	20.025	24.190		16.91 A
50											
50	ATOM	121	С	ILE		87	84.549	17.836	20.436		19.85 A
	ATOM	122	0	ILE		87	85.666	18.317	20.502		21.66 A
	ATOM	123	N	LEU		88	84.030	17.406	19.293		19.65 A
	ATOM	124	CA	LEU	Α	88	84.771	17.539	18.047	1.00	20.20 A
	ATOM	125	СВ	LEU	A	88	84.423	16.405	17.078	1.00	18.76 A
55	ATOM	126	CG	LEU	Α	88	84.807	14.981	17.493		16.99 A
	ATOM	127		LEU		88	84.122	13.995	16.570		13.92 A
	ATOM	128		LEU		88	86.305	14.809	17.441		11.51 A
	ATOM	129	C	LEU		88	84.429	18.861	17.407		20.87 A
	ATOM	130	0	LEU		88	85.233	19.443	16.709		21.48 A
	AION	100	\cup	∪نىر	А	5.0	00.400	17.113	10.703	1.00	21.70 A

	ATOM	131	N	GLY A	89	83.221	19.339	17.639	1.00 22.34 A
	ATOM	132	CA	GLY A	89	82.856	20.601	17.043	1.00 25.87 A
	ATOM	133	С	GLY A	89	81.476	21.057	17.451	1.00 29.45 A
	ATOM	134	0	GLY A	89	80.673	20.292	17.990	1.00 29.48 A
5	MOTA	135	N	GLU A	90	81.196	22.321	17.188	1.00 32.71 A
	ATOM	136	CA	GLU A	90	79.904	22.864	17.530	1.00 37.61 A
	ATOM	137	СВ	GLU A	90	80.047	23.798	18.738	1.00 38.05 A
	ATOM	138	CG	GLU A	90	80.123	22.998	20.037	1.00 42.04 A
	ATOM	139	CD	GLU A	90	80.463	23.813	21.270	1.00 45.47 A
10	ATOM	140	OE1	GLU A	90	81.662	24.137	21.477	1.00 47.26 A
	ATOM	141	OE2	GLU A	90	79.524	24.119	22.041	1.00 47.39 A
	ATOM	142	С	GLU A	90	79.277	23.565	16.349	1.00 40.01 A
	ATOM	143	0	GLU A	90	79.972	24.148	15.518	1.00 42.05 A
	ATOM	144	N	GLY A	91	77.962	23.440	16.240	1.00 42.05 A
15	ATOM	145	CA	GLY A	91	77.238	24.102	15.174	1.00 43.15 A
13									
	ATOM	146	С	GLY A	91	76.276	25.035	15.892	1.00 45.06 A
	ATOM	147	0	GLY A	91	76.317	25.149	17.134	1.00 43.58 A
	ATOM	148	N	SER A	92	75.408	25.699	15.136	1.00 46.66 A
		149		SER A	92	74.430	26.606	15.742	1.00 48.21 A
• •	ATOM		CA						
20	MOTA	150	СВ	SER A	92	73.754	27.462	14.660	1.00 51.13 A
	ATOM	151	OG	SER A	92	73.601	26.741	13.439	1.00 54.79 A
	ATOM	152	С	SER A	92	73.382	25.827	16.538	1.00 47.10 A
					92				1.00 49.44 A
	MOTA	153	0	SER A		73.055	26.190	17.678	
	MOTA	154	N	PHE A	93	72.874	24.743	15.957	1.00 44.39 A
25	ATOM	155	CA	PHE A	93	71.866	23.942	16.648	1.00 41.99 A
	ATOM	156	СВ	PHE A	93	70.617	23.798	15.780	1.00 43.92 A
		157	CG		93	70.434	24.919	14.814	1.00 47.66 A
	ATOM			PHE A					
	ATOM	158	CD1	PHE A	93	70.689	24.729	13.455	1.00 49.35 A
	ATOM	159	CD2	PHE A	93	70.061	26.185	15.264	1.00 49.16 A
30	ATOM	160	CE1	PHE A	93	70.581	25.789	12.551	1.00 51.11 A
20			CE2						
	ATOM	161		PHE A	93	69.949	27.257	14.374	1.00 50.58 A
	ATOM	162	CZ	PHE A	93	70.209	27.062	13.014	1.00 51.37 A
	ATOM	163	С	PHE A	93	72.352	22.555	17.028	1.00 38.35 A
	ATOM	164	0	PHE A	93	71.532	21.670	17.257	1.00 38.33 A
35							22.351		1.00 33.28 A
33	ATOM	165	N	SER A	94	73.665		17.106	
	MOTA	166	CA	SER A	94	74.151	21.028	17.440	1.00 29.57 A
	ATOM	167	CB	SER A	94	73.996	20.106	16.227	1.00 30.45 A
	ATOM	168	OG	SER A	94	75.123	20.190	15.368	1.00 30.51 A
	ATOM	169	C	SER A	94	75.588	20.952	17.936	1.00 27.66 A
40									
40	ATOM	170	0	SER A	94	76.369	21.893	17.803	1.00 27.25 A
	ATOM	171	N	THR A	95	75.927	19.807	18.512	1.00 25.06 A
	ATOM	172	CA	THR A	95	77.264	19.572	19.027	1.00 23.70 A
	ATOM	173	СВ	THR A	95	77.310	19.626	20.582	1.00 24.12 A
	MOTA	174		THR A	95	76.801	20.886	21.044	1.00 25.68 A
45	MOTA	175	CG2	THR A	95	78.731	19.458	21.073	1.00 22.92 A
	ATOM	176	С	THR A	95	77.655	18.180	18.594	1.00 22.05 A
	ATOM	177	0	THR A	95	76.860	17.250	18.673	1.00 21.43 A
	ATOM	178	N	VAL A	96	78.883	18.029	18.129	1.00 21.52 A
	MOTA	179	CA	VAL A	96	79.348	16.723	17.702	1.00 19.53 A
50	ATOM	180	CB	VAL A	96	79.980	16.818	16.316	1.00 19.24 A
	MOTA	181		VAL A	96	80.418	15.443	15.839	1.00 17.73 A
	ATOM	182		VAL A	96	78.983	17.442	15.353	1.00 18.03 A
	ATOM	183	С	VAL A	96	80.364	16.242	18.722	1.00 19.43 A
	ATOM	184	0	VAL A	96	81.372	16.910	18.959	1.00 19.84 A
55	ATOM	185	N	VAL A	97	80.099	15.082	19.324	1.00 17.90 A
55									
	ATOM	186	CA	VAL A	97	80.989	14.532	20.341	1.00 17.32 A
	ATOM	187	CB	VAL A	97	80.283	14.438	21.736	1.00 18.35 A
	ATOM	188	CG1	VAL A	97	79.581	15.750	22.066	1.00 20.10 A
	ATOM	189		VAL A	97	79.234	13.357	21.713	1.00 23.78 A
	111 01.1	100	002	417TI L7	<i>J</i> ,	, ,	10.007	-1.7	1.00 25.70 A

	MOTA	190	С	VAL A	97	81.471	13.144	19.949	1.00 17.15 A
	MOTA	191	0	VAL A	97	80.727	12.351	19.379	1.00 18.17 A
	ATOM	192	N	LEU A	98	82.735	12.866	20.243	1.00 17.34 A
_	ATOM	193	CA	LEU A		83.331	11.575	19.974	1.00 17.44 A
5	MOTA	194	СВ	LEU A		84.853	11.689	19.990	1.00 17.84 A
	ATOM	195	CG	LEU A	98	85.656	10.407	19.737	1.00 18.59 A
	ATOM	196	CD1	LEU A	98	85.259	9.803	18.387	1.00 18.87 A
	ATOM	197		LEU A		87.151	10.738	19.772	1.00 16.62 A
	ATOM	198	С	LEU A		82.874	10.626	21.081	1.00 18.35 A
10	ATOM	199	0	LEU A	98	82.992	10.926	22.259	1.00 18.60 A
	MOTA	200	N	ALA A	99	82.340	9.476	20.697	1.00 19.15 A
	ATOM	201	CA	ALA A	99	81.888	8.513	21.675	1.00 19.73 A
	ATOM	202	СВ	ALA A		80.383	8.534	21.759	1.00 17.97 A
	ATOM	203	С	ALA A		82.360	7.117	21.317	1.00 21.86 A
15	ATOM	204	0	ALA A	99	82.502	6.766	20.131	1.00 22.18 A
	ATOM	205	N	ARG A	100	82.631	6.324	22.345	1.00 21.93 A
	ATOM	206	CA	ARG A	100	83.025	4.963	22.102	1.00 23.29 A
	ATOM	207	СВ	ARG A		84.333	4.637	22.805	1.00 25.99 A
	ATOM	208	CG	ARG A		84.870	3.271	22.388	1.00 31.56 A
20	ATOM	209	CD	ARG A	100	86.146	2.923	23.129	1.00 35.19 A
	ATOM	210	NE	ARG A	100	87.220	3.875	22.847	1.00 37.39 A
	ATOM	211	CZ	ARG A	100	87.958	3.870	21.740	1.00 38.05 A
	ATOM	212		ARG A		87.742	2.953	20.797	1.00 37.25 A
	ATOM	213		ARG A		88.918	4.780	21.580	1.00 36.22 A
25	MOTA	214	С	ARG A	100	81.904	4.060	22.603	1.00 22.07 A
	ATOM	215	0	ARG A	100	81.460	4.177	23.743	1.00 22.10 A
	ATOM	216	N	GLU A	101	81.417	3.189	21.734	1.00 21.29 A
	ATOM	217	CA	GLU A		80.357	2.262	22.119	1.00 22.87 A
• •	ATOM	218	СВ	GLU A		79.747	1.631	20.867	1.00 23.10 A
30	ATOM	219	CG	GLU A	101	78.740	0.563	21.148	1.00 22.71 A
	ATOM	220	CD	GLU A	101	78.128	0.040	19.878	1.00 23.56 A
	ATOM	221	OE1	GLU A	101	78.892	-0.198	18.922	1.00 21.84 A
	ATOM	222	OE2	GLU A		76.890	-0.143	19.832	1.00 26.29 A
	ATOM	223	С	GLU A		80.942	1.176	23.037	1.00 21.56 A
35	ATOM	224	0	GLU A	101	81.884	0.485	22.666	1.00 20.69 A
	ATOM	225	N	LEU A	102	80.389	1.042	24.236	1.00 21.11 A
	ATOM	226	CA	LEU A	102	80.874	0.057	25.204	1.00 21.54 A
	ATOM	227	СВ	LEU A		80.075	0.199	26.507	1.00 20.90 A
4.0	ATOM	228	CG	LEU A		80.193	1.620	27.092	1.00 22.35 A
40	MOTA	229		LEU A		79.177	1.798	28.207	1.00 20.18 A
	MOTA	230	CD2	LEU A	102	81.600	1.866	27.608	1.00 17.47 A
	ATOM	231	С	LEU A	102	80.896	-1.415	24.729	1.00 20.27 A
	ATOM	232	0	LEU A		81.922	-2.078		1.00 21.63 A
	ATOM	233	N	ALA A		79.792			1.00 18.37 A
15									
45	ATOM	234	CA	ALA A		79.757	-3.307	23.731	1.00 20.54 A
	MOTA	235	СВ	ALA A	103	78.333	-3.694	23.359	1.00 19.31 A
	ATOM	236	С	ALA A	103	80.688	-3.658	22.552	1.00 22.26 A
	ATOM	237	0	ALA A	103	81.002	-4.829	22.358	1.00 23.93 A
	ATOM	238	N	THR A		81.141	-2.677	21.775	1.00 20.79 A
50									
50	ATOM	239	CA	THR A		81.972	-2.999	20.622	1.00 21.40 A
	MOTA	240	СВ	THR A	104	81.279	-2.632	19.326	1.00 20.97 A
	ATOM	241	OG1	THR A	104	81.174	-1.205	19.259	1.00 23.21 A
	ATOM	242		THR A		79.891	-3.266	19.245	1.00 19.82 A
		243	C					20.569	
	ATOM			THR A		83.304	-2.300		1.00 23.57 A
55	ATOM	244	0	THR A		84.168	-2.687	19.796	1.00 23.41 A
	ATOM	245	N	SER A	105	83.454	-1.243	21.359	1.00 24.64 A
	ATOM	246	CA	SER A	105	84.687	-0.487	21.390	1.00 24.23 A
	ATOM	247	СВ	SER A		85.855	-1.467	21.481	1.00 25.40 A
			OG			87.074	-0.788		
	ATOM	248	UG	SER A	103	0/.0/4	-0.700	21.719	1.00 34.15 A

	ATOM	249	С	SER A	105	84.819	0.454	20.163	1.00 23.42 A
	ATOM	250	0	SER A	105	85.803	1.187	20.013	1.00 23.28 A
	ATOM	251	N	ARG A	106	83.821	0.448	19.295	1.00 21.19 A
	ATOM	252	CA	ARG A		83.850	1.323	18.115	1.00 22.25 A
5	ATOM	253	СВ	ARG A		82.754	0.922	17.118	1.00 24.82 A
5									
	MOTA	254	CG	ARG A		83.027	-0.343	16.349	1.00 25.20 A
	ATOM	255	CD	ARG A	106	81.740	-0.942	15.884	1.00 25.19 A
	MOTA	256	NE	ARG A	106	81.972	-1.900	14.815	1.00 26.11 A
	ATOM	257	CZ	ARG A	106	81.042	-2.707	14.322	1.00 24.24 A
10	ATOM	258	NH1	ARG A		79.805	-2.677	14.818	1.00 21.06 A
	ATOM	259		ARG A		81.351	-3.513	13.315	1.00 20.25 A
	ATOM	260	С	ARG A		83.655	2.806	18.433	1.00 19.79 A
	ATOM	261	0	ARG A		82.836	3.175	19.266	1.00 18.73 A
	MOTA	262	N	GLU A	107	84.404	3.646	17.736	1.00 19.82 A
15	ATOM	263	CA	GLU A	107	84.294	5.086	17.903	1.00 21.14 A
	ATOM	264	СВ	GLU A		85.656	5.746	17.777	1.00 21.88 A
	ATOM	265	CG	GLU A		86.562	5.428	18.926	1.00 26.09 A
									1.00 20.09 A
	ATOM	266	CD	GLU A		87.916	6.043	18.746	
	MOTA	267		GLU A		88.212	7.057	19.434	1.00 32.48 A
20	MOTA	268	OE2	GLU A	107	88.678	5.512	17.901	1.00 31.98 A
	MOTA	269	С	GLU A	107	83.358	5.693	16.870	1.00 20.50 A
	ATOM	270	0	GLU A	107	83.474	5.429	15.676	1.00 20.70 A
	ATOM	271	N	TYR A	108	82.415	6.498	17.347	1.00 20.38 A
	ATOM	272	CA	TYR A		81.464	7.172	16.477	1.00 18.49 A
25	ATOM	273	CB	TYR A		80.049	6.660	16.700	1.00 10.19 A
23		274		TYR A					
	ATOM		CG			79.828	5.247	16.238	1.00 23.37 A
	MOTA	275	CD1	TYR A		79.598	4.964	14.886	1.00 22.79 A
	MOTA	276	CE1	TYR A		79.357	3.648	14.458	1.00 23.56 A
	MOTA	277	CD2	TYR A	108	79.820	4.180	17.154	1.00 21.34 A
30	MOTA	278	CE2	TYR A	108	79.583	2.873	16.740	1.00 20.43 A
	ATOM	279	CZ	TYR A	108	79.346	2.609	15.392	1.00 23.44 A
	ATOM	280	OH	TYR A	108	79.061	1.321	14.972	1.00 24.10 A
	ATOM	281	С	TYR A		81.478	8.635	16.828	1.00 18.53 A
	ATOM	282	0	TYR A		81.778	9.011	17.971	1.00 17.37 A
35	ATOM	283	N	ALA A		81.169	9.453	15.829	1.00 17.24 A
33									
	MOTA	284	CA	ALA A		81.053	10.885	16.006	1.00 15.98 A
	MOTA	285	СВ	ALA A		81.597	11.600	14.788	1.00 15.20 A
	MOTA	286	С	ALA A	109	79.528	11.087	16.140	1.00 15.73 A
	MOTA	287	0	ALA A	109	78.767	10.873	15.191	1.00 15.79 A
40	ATOM	288	N	ILE A	110	79.070	11.474	17.320	1.00 14.95 A
	ATOM	289	CA	ILE A		77.636	11.636	17.511	1.00 15.99 A
	ATOM	290	СВ	ILE A		77.188	10.940	18.815	1.00 15.51 A
	ATOM	291		ILE A		75.697	11.126	19.039	
4.5	MOTA	292		ILE A			9.452	18.729	1.00 16.63 A
45	ATOM	293	CDI	ILE A		76.964	8.595	19.847	1.00 16.83 A
	MOTA	294	С	ILE A	110	77.176	13.085	17.514	1.00 16.55 A
	MOTA	295	0	ILE A	110	77.583	13.873	18.370	1.00 16.24 A
	ATOM	296	N	LYS A	111	76.343	13.430	16.538	1.00 16.03 A
	ATOM	297	CA	LYS A	111	75.804	14.777	16.430	1.00 18.21 A
50	ATOM	298	СВ	LYS A		75.341	15.065	14.997	1.00 19.36 A
50		299	CG			75.035	16.548		1.00 22.68 A
	ATOM			LYS A				14.768	
	MOTA	300	CD	LYS A		74.461	16.844	13.396	1.00 23.67 A
	ATOM	301	CE	LYS A		74.876	18.222	12.930	1.00 23.18 A
	MOTA	302	NZ	LYS A	111	73.744	18.938	12.304	1.00 28.83 A
55	ATOM	303	С	LYS A	111	74.608	14.866	17.383	1.00 17.40 A
	ATOM	304	0	LYS A		73.646	14.115	17.239	1.00 18.27 A
	ATOM	305	N	ILE A		74.672	15.781	18.344	1.00 15.41 A
	ATOM	306	CA	ILE A		73.609	15.938	19.331	1.00 16.56 A
		307	CB						1.00 10.30 A
	ATOM	307	CD	ILE A	114	74.194	15.819	20.777	1.00 11.09 A

	ATOM	308	CG2	ILE	Α	112	73.073	15.926	21.830	1.00	11.60	Α
	ATOM	309	CG1				74.957	14.480	20.885	1.00	16.81	Α
	ATOM	310	CD1				75.771	14.262	22.178		15.96	
	ATOM	311	C	ILE			72.876	17.261	19.158		17.98	
5	ATOM	312	0	ILE			73.504	18.314	18.965		16.70	
5				LEU			71.546		19.195		19.61	
	ATOM	313	N					17.198				
	ATOM	314	CA	LEU			70.711	18.393	19.034		21.99	
	ATOM	315	СВ	LEU			70.058	18.434	17.641		22.17	
	ATOM	316	CG	LEU	A	113	70.906	18.273	16.367		22.83	
10	ATOM	317	CD1	LEU	Α	113	71.124	16.792	16.059		22.72	
	ATOM	318	CD2	LEU	Α	113	70.191	18.912	15.206	1.00	21.97	Α
	ATOM	319	С	LEU	Α	113	69.612	18.419	20.088	1.00	24.22	Α
	ATOM	320	0	LEU	Α	113	69.062	17.378	20.469	1.00	24.61	Α
	ATOM	321	N	GLU	Α	114	69.285	19.615	20.559	1.00	27.06	Α
15	ATOM	322	CA	GLU			68.247	19.759	21.567	1.00	28.93	Α
	ATOM	323	СВ	GLU			68.586	20.926	22.488		31.39	
	ATOM	324	CG	GLU			67.671	21.026	23.684		39.92	
	ATOM	325	CD	GLU			67.676	22.406	24.300		45.42	
	ATOM	326		GLU			67.160	23.356	23.655		46.90	
20		327	OE 2	GLU			68.204	22.540	25.429			
20	ATOM										50.09	
	ATOM	328	C	GLU			66.887	19.978	20.892		29.21	
	ATOM	329	0	GLU			66.679	20.969	20.177		29.53	
	ATOM	330	N	LYS			65.962	19.051	21.116		28.74	
	ATOM	331	CA	LYS			64.642	19.152	20.507		29.44	
25	ATOM	332	СВ	LYS			63.744	18.002	20.987		28.12	
	ATOM	333	CG	LYS			63.827	16.758	20.103		28.47	
	ATOM	334	CD	LYS	Α	115	63.026	15.571	20.639		27.07	
	MOTA	335	CE	LYS	Α	115	63.738	14.854	21.779	1.00	28.88	Α
	ATOM	336	NZ	LYS	Α	115	62.963	13.672	22.282	1.00	26.42	Α
30	ATOM	337	С	LYS	Α	115	63.947	20.502	20.724	1.00	29.72	Α
	ATOM	338	0	LYS			63.310	21.025	19.799	1.00	30.03	Α
	ATOM	339	N	ALA			64.082	21.091	21.910		28.83	
	ATOM	340	CA	ALA			63.407	22.365	22.159		29.91	
	ATOM	341	СВ	ALA			63.470	22.749	23.647		28.16	
35	ATOM	342	C	ALA			63.976	23.480	21.311		30.93	
55	ATOM	343	0	ALA			63.231	24.217	20.667		32.28	
	ATOM	344	N	HIS			65.297	23.593	21.292		31.66	
		345	CA	HIS			65.951	24.645	20.523		32.13	
	ATOM ATOM	346	CB	HIS			67.472	24.571	20.728		34.12	
40								25.741			37.74	
40	ATOM	347	CG	HIS			68.219		20.169			
	ATOM	348		HIS			67.794	26.959	19.761		39.67	
	ATOM	349		HIS			69.582	25.727	19.966		42.04	
	ATOM	350		HIS			69.965	26.884	19.454		41.07	
	ATOM	351		HIS			68.899	27.649	19.320		40.56	
45	ATOM	352	С	HIS			65.600	24.547	19.040		31.36	
	ATOM	353	0	HIS	A	117	65.466	25.560	18.350		32.37	
	ATOM	354	N	ILE	Α	118	65.430	23.330	18.544	1.00	30.26	Α
	ATOM	355	CA	ILE	Α	118	65.102	23.158	17.132	1.00	29.28	Α
	ATOM	356	СВ	ILE	Α	118	65.266	21.696	16.712	1.00	27.64	Α
50	ATOM	357	CG2	ILE	Α	118	64.560	21.439	15.401	1.00	22.46	Α
	ATOM	358	CG1	ILE	Α	118	66.756	21.371	16.642	1.00	27.22	Α
	ATOM	359	CD1	ILE	Α	118	67.036	19.917	16.437	1.00	30.51	Α
	ATOM	360	С	ILE			63.688	23.618	16.816		30.41	
	ATOM	361	0	ILE			63.444	24.251	15.785		29.55	
55	ATOM	362	N	ILE			62.756	23.291	17.705		29.59	
	ATOM	363	CA	ILE			61.376	23.682	17.497		29.18	
	ATOM	364	CB	ILE			60.447	22.979	18.506		27.15	
	ATOM	365		ILE			59.071	23.623	18.486		22.69	
	ATOM	366	CGI	ILE	А	ттэ	60.394	21.486	18.173	1.00	23.45	А

	MOTA	367	CD1	ILE A	. 119	59.666	20.665	19.173	1.00 19.08 A
	ATOM	368	С	ILE A	. 119	61.223	25.194	17.617	1.00 30.65 A
	ATOM	369	0	ILE A		60.574	25.832	16.786	1.00 30.59 A
_	ATOM	370	N	ALA A		61.837	25.768	18.642	1.00 31.95 A
5	MOTA	371	CA	ALA A	. 120	61.752	27.205	18.848	1.00 33.69 A
	ATOM	372	СВ	ALA A	. 120	62.473	27.608	20.150	1.00 33.17 A
	ATOM	373	С	ALA A	. 120	62.330	27.973	17.671	1.00 34.80 A
	ATOM	374	0	ALA A		61.865	29.067	17.362	1.00 37.34 A
10	ATOM	375	N	GLU A		63.328	27.413	16.997	1.00 35.09 A
10	ATOM	376	CA	GLU A	. 121	63.941	28.116	15.872	1.00 35.31 A
	ATOM	377	СВ	GLU A	. 121	65.453	27.927	15.933	1.00 39.72 A
	ATOM	378	CG	GLU A	121	66.103	28.735	17.038	1.00 45.91 A
	ATOM	379	CD	GLU A		65.955	30.225	16.784	1.00 49.51 A
	ATOM	380		GLU A		66.634	30.736	15.866	1.00 52.87 A
15	ATOM	381	OE2	GLU A		65.148	30.879	17.482	1.00 51.35 A
	ATOM	382	С	GLU A	. 121	63.421	27.699	14.499	1.00 34.14 A
	ATOM	383	0	GLU A	121	63.964	28.109	13.468	1.00 31.41 A
	ATOM	384	N	ASN A		62.363	26.891	14.497	1.00 33.86 A
• •	ATOM	385	CA	ASN A		61.771	26.367	13.266	1.00 34.00 A
20	ATOM	386	СВ	ASN A	. 122	61.112	27.473	12.464	1.00 36.75 A
	ATOM	387	CG	ASN A	. 122	59.962	28.081	13.193	1.00 39.62 A
	ATOM	388	OD1	ASN A	122	60.148	28.788	14.185	1.00 39.90 A
	ATOM	389		ASN A		58.753	27.794	12.727	1.00 41.02 A
									1.00 41.02 A 1.00 31.78 A
	ATOM	390	С	ASN A		62.798	25.686	12.397	
25	ATOM	391	0	ASN A		62.958	26.035	11.230	1.00 32.05 A
	MOTA	392	N	LYS A	. 123	63.494	24.714	12.965	1.00 28.71 A
	ATOM	393	CA	LYS A	. 123	64.508	24.008	12.217	1.00 29.39 A
	ATOM	394	СВ	LYS A	123	65.842	24.036	12.974	1.00 31.70 A
	ATOM	395	CG	LYS A		66.434	25.416	13.132	1.00 33.49 A
20									
30	ATOM	396	CD	LYS A		66.612	26.076	11.763	1.00 37.43 A
	MOTA	397	CE	LYS A	. 123	67.174	27.491	11.898	1.00 38.52 A
	ATOM	398	NZ	LYS A	. 123	67.337	28.176	10.582	1.00 37.85 A
	ATOM	399	С	LYS A	123	64.116	22.572	11.931	1.00 28.30 A
	ATOM	400	0	LYS A		64.867	21.844	11.289	1.00 29.68 A
25									
35	ATOM	401	N	VAL A		62.944	22.162	12.404	1.00 26.80 A
	ATOM	402	CA	VAL A		62.484	20.796	12.175	1.00 26.73 A
	MOTA	403	CB	VAL A	. 124	61.024	20.593	12.622	1.00 26.31 A
	ATOM	404	CG1	VAL A	. 124	60.532	19.222	12.191	1.00 25.31 A
	ATOM	405	CG2	VAL A	124	60.918	20.720	14.134	1.00 26.73 A
40	ATOM	406	C	VAL A		62.594	20.351	10.722	1.00 27.11 A
40									
	ATOM	407	0	VAL A		62.973	19.218	10.450	1.00 29.79 A
	ATOM	408	N	PRO A	. 125	62.270	21.228	9.763	1.00 27.28 A
	ATOM	409	CD	PRO A	. 125	61.610	22.544	9.818	1.00 27.49 A
	ATOM	410	CA	PRO A	. 125	62.386	20.758	8.378	1.00 27.41 A
45	ATOM	411	СВ	PRO A		61.775	21.904	7.563	1.00 26.08 A
15									
	ATOM	412	CG	PRO A		60.821	22.546	8.524	1.00 27.54 A
	ATOM	413	С	PRO A	. 125	63.837	20.506	8.006	1.00 27.90 A
	MOTA	414	0	PRO A	. 125	64.162	19.572	7.260	1.00 26.27 A
	ATOM	415	N	TYR A	. 126	64.703	21.350	8.550	1.00 28.64 A
50	ATOM	416	CA	TYR A		66.123	21.271	8.288	1.00 30.11 A
50								8.809	
	ATOM	417	СВ	TYR A		66.791	22.528		1.00 36.70 A
	ATOM	418	CG	TYR A		66.440	23.774	8.013	1.00 44.64 A
	MOTA	419	CD1	TYR A	. 126	66.984	23.988	6.744	1.00 47.43 A
	ATOM	420	CE1	TYR A	. 126	66.737	25.173	6.037	1.00 50.16 A
55	ATOM	421		TYR A		65.620	24.774	8.557	1.00 47.03 A
55									
	ATOM	422		TYR A		65.369	25.955	7.861	1.00 49.52 A
	ATOM	423	CZ	TYR A		65.936	26.152	6.605	1.00 50.60 A
	ATOM	424	OH	TYR A	. 126	65.754	27.349	5.941	1.00 52.77 A
	ATOM	425	С	TYR A	. 126	66.794	20.041	8.874	1.00 28.69 A

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	ATOM	426	0	TYR A	. 126	67.613	19.407	8.208	1.00 28.32	А
	ATOM	427	N	VAL A	. 127	66.464	19.714	10.118	1.00 25.64	Α
	ATOM	428	CA	VAL A	127	67.033	18.550	10.766	1.00 24.89	Α
	ATOM	429	СВ	VAL A		66.664	18.513	12.258	1.00 26.70	
_										
5	ATOM	430		VAL A		67.158	17.206	12.881	1.00 22.51	
	ATOM	431	CG2	VAL A	. 127	67.255	19.743	12.972	1.00 23.84	Α
	ATOM	432	С	VAL A	127	66.521	17.276	10.097	1.00 24.81	Α
		433		VAL A		67.260	16.315	9.890	1.00 24.02	
	ATOM		0							
	ATOM	434	N	THR A	. 128	65.245	17.290	9.755	1.00 24.02	Α
10	ATOM	435	CA	THR A	. 128	64.608	16.164	9.088	1.00 24.59	Α
	ATOM	436	СВ	THR A	128	63.123	16.471	8.843	1.00 25.38	Z
	ATOM	437		THR A		62.478	16.652	10.106	1.00 25.76	
	MOTA	438	CG2	THR A	. 128	62.451	15.354	8.066	1.00 22.88	Α
	ATOM	439	С	THR A	. 128	65.266	15.875	7.744	1.00 24.53	Α
15	ATOM	440	0	THR A		65.560	14.729	7.426	1.00 25.53	
13										
	ATOM	441	N	ARG A		65.477	16.925	6.957	1.00 24.82	
	ATOM	442	CA	ARG A	. 129	66.099	16.812	5.646	1.00 25.49	Α
	ATOM	443	СВ	ARG A	. 129	66.111	18.181	4.959	1.00 26.78	Α
	ATOM	444	CG	ARG A		66.648	18.175	3.529	1.00 32.33	
20										
20	ATOM	445	CD	ARG A		66.579	19.563	2.878	1.00 36.93	
	ATOM	446	NE	ARG A	. 129	65.326	20.249	3.184	1.00 42.70	Α
	ATOM	447	CZ	ARG A	. 129	65.254	21.462	3.730	1.00 46.67	Α
	ATOM	448		ARG A		66.366	22.128	4.018	1.00 48.50	
	ATOM	449	NH2	ARG A		64.073	21.997	4.027	1.00 48.90	
25	ATOM	450	С	ARG A	. 129	67.532	16.296	5.801	1.00 26.46	Α
	ATOM	451	0	ARG A	. 129	68.002	15.456	5.020	1.00 24.76	Α
	ATOM	452	N	GLU A		68.216	16.795	6.825	1.00 25.56	Δ
	ATOM	453	CA	GLU A		69.582	16.393	7.076	1.00 28.29	
	ATOM	454	СВ	GLU A	. 130	70.118	17.106	8.310	1.00 27.95	Α
30	ATOM	455	CG	GLU A	. 130	71.591	16.875	8.539	1.00 29.48	Α
	ATOM	456	CD	GLU A		72.107	17.566	9.787	1.00 32.14	
	ATOM	457		GLU A		71.297	18.221	10.483	1.00 32.67	
	ATOM	458	OE2	GLU A	. 130	73.325	17.450	10.069	1.00 32.21	Α
	ATOM	459	С	GLU A	130	69.665	14.886	7.279	1.00 29.86	Α
35	ATOM	460	0	GLU A		70.498	14.200	6.668	1.00 29.35	
33										
	MOTA	461	N	ARG A		68.797	14.382	8.150	1.00 30.84	
	ATOM	462	CA	ARG A	. 131	68.763	12.966	8.451	1.00 31.62	Α
	ATOM	463	СВ	ARG A	. 131	67.786	12.684	9.598	1.00 33.12	Α
	ATOM	464	CG	ARG A		67.557	11.190	9.831	1.00 36.17	
40							10.925		1.00 41.69	
40	ATOM	465	CD	ARG A		66.560		10.946		
	MOTA	466	NE	ARG A	. 131	66.330	9.492	11.166	1.00 46.62	Α
	ATOM	467	CZ	ARG A	. 131	65.692	8.986	12.224	1.00 48.29	Α
	ATOM	468	NH1	ARG A	131	65.215	9.795	13.165	1.00 49.51	Α
	ATOM	469		ARG A		65.544	7.671	12.352	1.00 48.76	
4.5										
45	ATOM	470	С	ARG A	. 131	68.371	12.138	7.235	1.00 30.59	
	ATOM	471	0	ARG A	. 131	68.897	11.051	7.026	1.00 29.96	Α
	ATOM	472	N	ASP A	132	67.446	12.649	6.433	1.00 29.54	Δ
		473	CA	ASP A		67.000	11.913	5.259	1.00 29.40	
	ATOM									
	ATOM	474	СВ	ASP A	. 132	65.735	12.565	4.708	1.00 32.43	
50	ATOM	475	CG	ASP A	. 132	64.531	12.395	5.655	1.00 38.15	Α
	ATOM	476	OD1	ASP A	132	64.749	12.227	6.881	1.00 40.40	Α
	ATOM					63.365			1.00 41.19	
		477		ASP A			12.439	5.186		
	ATOM	478	С	ASP A		68.088	11.789	4.189	1.00 27.62	
	ATOM	479	0	ASP A	. 132	68.232	10.744	3.553	1.00 26.54	Α
55	ATOM	480	N	VAL A		68.862	12.850	4.011	1.00 25.14	
				VAL A					1.00 24.12	
	ATOM	481	CA			69.939	12.857	3.044		
	ATOM	482	СВ	VAL A		70.451	14.272	2.833	1.00 24.07	
	ATOM	483	CG1	VAL A	. 133	71.802	14.247	2.143	1.00 23.77	Α
	ATOM	484	CG2	VAL A	. 133	69.461	15.030	2.008	1.00 24.30	

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	ATOM	485	С	VAL 2			71.099	11.975	3.504		24.97	
	ATOM	486	0	VAL 2			71.672	11.221	2.712	1.00	24.95	Α
	ATOM	487	N	MET 2	A	134	71.458	12.074	4.779	1.00	23.41	Α
	ATOM	488	CA	MET 2	A	134	72.539	11.255	5.268	1.00	23.12	Α
5	ATOM	489	СВ	MET 2			72.932	11.653	6.683		21.12	
5		490		MET 2				13.005	6.759		21.21	
	ATOM		CG				73.608					
	ATOM	491	SD	MET 2	A	134	74.530	13.204	8.291		20.52	
	ATOM	492	CE	MET 2	A	134	73.172	13.347	9.534	1.00	17.71	Α
	ATOM	493	С	MET 2	A	134	72.163	9.783	5.237	1.00	24.75	Α
10	ATOM	494	0	MET 2	Δ	134	73.027	8.918	5.039		25.73	
10	ATOM	495	N	SER I			70.885	9.474	5.425		23.96	
	ATOM	496	CA	SER 2			70.484	8.064	5.408		24.82	
	ATOM	497	СВ	SER I	A	135	69.048	7.889	5.917	1.00	24.63	Α
	ATOM	498	OG	SER I	Α	135	68.139	8.496	5.015	1.00	29.80	Α
15	ATOM	499	С	SER 2	Α	135	70.585	7.479	4.003	1.00	22.35	Α
	ATOM	500	0	SER .			70.534	6.274	3.829		21.60	
		501		ARG 2			70.729	8.335	3.004		21.91	
	ATOM		N									
	ATOM	502	CA	ARG 2			70.815	7.858	1.631		23.76	
	ATOM	503	СВ	ARG 2	A	136	69.988	8.762	0.714	1.00	25.55	Α
20	ATOM	504	CG	ARG 2	Α	136	68.500	8.782	1.069	1.00	31.38	Α
	ATOM	505	CD	ARG 2	A	136	67.764	9.897	0.332	1.00	33.65	Α
	ATOM	506	NE	ARG 2			68.024	9.809	-1.099		38.77	
											41.27	
	ATOM	507	CZ	ARG 2			67.654	10.718	-1.996			
	ATOM	508		ARG 2			66.988	11.806	-1.604		42.53	
25	ATOM	509	NH2	ARG 2	A	136	67.971	10.544	-3.286	1.00	39.41	Α
	ATOM	510	С	ARG 2	Α	136	72.248	7.789	1.131	1.00	22.64	Α
	ATOM	511	0	ARG 2			72.520	7.268	0.052	1.00	22.43	Α
	ATOM	512	N	LEU I			73.168	8.318	1.919		22.66	
• •	ATOM	513	CA	LEU 2			74.568	8.307	1.535		22.60	
30	ATOM	514	СВ	LEU 2			75.348	9.375	2.308		20.28	
	ATOM	515	CG	LEU 2	A	137	74.842	10.793	2.068	1.00	19.72	Α
	ATOM	516	CD1	LEU 2	Α	137	75.695	11.816	2.840	1.00	17.83	Α
	ATOM	517	CD2	LEU 2	Α	137	74.855	11.062	0.564	1.00	18.39	Α
	ATOM	518	C	LEU I			75.195	6.950	1.775		22.60	
25												
35	ATOM	519	0	LEU Z			75.203	6.445	2.892		23.75	
	MOTA	520	N	ASP I			75.723	6.371	0.710		22.09	
	ATOM	521	CA	ASP 2	A	138	76.383	5.083	0.788	1.00	22.63	Α
	ATOM	522	CB	ASP I	A	138	75.419	3.988	0.340	1.00	25.16	Α
	ATOM	523	CG	ASP I	A	138	75.976	2.622	0.582	1.00	26.26	Α
40	ATOM	524		ASP 2			76.658	2.480	1.611		27.29	
40		525		ASP I			75.740		-0.237		30.75	
	ATOM							1.708				
	MOTA	526	С	ASP I			77.617	5.112	-0.124		20.82	
	ATOM	527	0	ASP I	A	138	77.656	4.445	-1.155	1.00	22.94	Α
	ATOM	528	N	HIS 2	A	139	78.612	5.902	0.250	1.00	16.77	Α
45	ATOM	529	CA	HIS I	A	139	79.813	6.050	-0.557	1.00	16.21	Α
	ATOM	530	СВ	HIS I			79.614	7.180	-1.583		15.30	
	ATOM	531	CG	HIS I			80.755	7.348	-2.534		16.37	
	MOTA	532		HIS I			80.853	7.087	-3.860		15.32	
	ATOM	533	ND1	HIS 2	A	139	81.998	7.802	-2.139	1.00	17.12	Α
50	ATOM	534	CE1	HIS I	Α	139	82.811	7.810	-3.184	1.00	15.92	Α
	ATOM	535	NE2	HIS 2	A	139	82.140	7.380	-4.238	1.00	13.96	Α
	ATOM	536	С	HIS I			80.985	6.371	0.357		16.70	
	ATOM	537	0	HIS I			80.848	7.116	1.317		16.89	
	ATOM	538	N	PRO 1	A	140	82.164	5.823	0.056		16.94	
55	ATOM	539	CD	PRO 2	A	140	82.508	4.991	-1.108	1.00	17.10	Α
	ATOM	540	CA	PRO 2	A	140	83.334	6.079	0.895	1.00	17.98	Α
	ATOM	541	СВ	PRO 2			84.390	5.163	0.291		17.03	
	ATOM	542	CG	PRO I			84.003	5.114	-1.159		18.59	
	ATOM	543	С	PRO 2	Α	14U	83.822	7.528	1.070	T.00	18.59	А

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	ATOM	544	0	PRO A		84.528	7.817	2.021	1.00 20.11 A
	ATOM	545	N	PHE A	141	83.460	8.444	0.179	1.00 19.62 A
	ATOM	546	CA	PHE A	141	83.909	9.833	0.345	1.00 18.34 A
	ATOM	547	СВ	PHE A	141	84.223	10.474	-1.010	1.00 17.53 A
5	ATOM	548	CG	PHE A		85.440	9.880	-1.694	1.00 17.38 A
5		549		PHE A		86.450	9.275	-0.938	1.00 17.30 A
	ATOM								
	ATOM	550	CD2	PHE A	141	85.579	9.926	-3.081	1.00 15.76 A
	ATOM	551	CE1	PHE A	141	87.572	8.724	-1.550	1.00 16.13 A
	ATOM	552	CE2	PHE A	141	86.707	9.375	-3.708	1.00 16.99 A
10	ATOM	553	CZ	PHE A	. 141	87.705	8.772	-2.938	1.00 15.01 A
	ATOM	554	C	PHE A		82.893	10.680	1.095	1.00 18.14 A
	ATOM	555	0	PHE A		83.012	11.896	1.144	1.00 20.74 A
	ATOM	556	N	PHE A		81.901	10.037	1.697	1.00 15.85 A
	ATOM	557	CA	PHE A	142	80.887	10.761	2.444	1.00 15.95 A
15	ATOM	558	СВ	PHE A	142	79.558	10.757	1.690	1.00 15.20 A
	ATOM	559	CG	PHE A		79.507	11.721	0.542	1.00 15.62 A
	ATOM	560		PHE A		79.295	13.086	0.768	1.00 14.51 A
	ATOM	561		PHE A		79.651	11.265	-0.771	1.00 12.05 A
	ATOM	562	CE1	PHE P	142	79.222	13.991	-0.291	1.00 13.97 A
20	ATOM	563	CE2	PHE A	142	79.582	12.157	-1.840	1.00 15.46 A
	ATOM	564	CZ	PHE A	142	79.365	13.536	-1.601	1.00 14.89 A
	ATOM	565	С	PHE A		80.654	10.167	3.824	1.00 15.60 A
									1.00 15.30 A
	ATOM	566	0	PHE A		80.886	8.986	4.061	
	ATOM	567	N	VAL A		80.182	11.001	4.733	1.00 15.87 A
25	ATOM	568	CA	VAL A	143	79.878	10.564	6.075	1.00 15.04 A
	ATOM	569	СВ	VAL A	143	79.304	11.727	6.905	1.00 15.26 A
	ATOM	570	CG1	VAL A	143	78.012	12.231	6.276	1.00 11.03 A
	ATOM	571		VAL A		79.100	11.296	8.350	1.00 14.40 A
20	ATOM	572	С	VAL A		78.828	9.479	5.935	1.00 15.52 A
30	ATOM	573	0	VAL A		78.076	9.453	4.963	1.00 15.45 A
	ATOM	574	N	LYS A	144	78.794	8.580	6.907	1.00 16.29 A
	ATOM	575	CA	LYS A	144	77.848	7.482	6.933	1.00 17.45 A
	ATOM	576	СВ	LYS A	144	78.625	6.150	6.895	1.00 18.05 A
	ATOM	577	CG	LYS A		77.963	4.967	7.596	1.00 24.34 A
35		578		LYS A		76.922	4.263	6.752	1.00 26.35 A
33	ATOM		CD						
	ATOM	579	CE	LYS A		77.461	2.926	6.213	1.00 30.22 A
	ATOM	580	NZ	LYS A	144	77.576	1.882	7.271	1.00 28.27 A
	ATOM	581	С	LYS A	144	77.024	7.626	8.222	1.00 17.39 A
	ATOM	582	0	LYS A	144	77.565	7.913	9.284	1.00 16.92 A
40	ATOM	583	N	LEU A	145	75.711	7.458	8.116	1.00 17.41 A
	ATOM	584	CA	LEU A		74.836	7.549	9.274	1.00 18.13 A
	ATOM	585	CB	LEU A		73.514	8.210	8.893	1.00 18.86 A
	MOTA	586	CG	LEU A		72.612	8.850	9.964	1.00 20.13 A
	ATOM	587	CD1	LEU A	145	71.157	8.607	9.582	1.00 19.48 A
45	ATOM	588	CD2	LEU A	145	72.900	8.311	11.331	1.00 17.86 A
	ATOM	589	С	LEU A	145	74.559	6.113	9.689	1.00 18.85 A
	ATOM	590	0	LEU A		73.905	5.379	8.954	1.00 20.15 A
		591	N			75.030	5.713	10.867	1.00 18.09 A
	ATOM			TYR A					
	ATOM	592	CA	TYR A		74.830	4.341	11.329	1.00 15.93 A
50	ATOM	593	СВ	TYR A	146	76.013	3.871	12.154	1.00 14.52 A
	ATOM	594	CG	TYR A	146	77.295	3.776	11.390	1.00 13.98 A
	ATOM	595	CD1	TYR A	146	78.093	4.907	11.193	1.00 15.01 A
	ATOM	596		TYR A		79.329	4.815	10.548	1.00 14.94 A
							2.541	10.912	1.00 14.36 A
55	ATOM	597		TYR A		77.752			
55	ATOM	598		TYR A		78.984	2.426	10.266	1.00 15.47 A
	ATOM	599	CZ	TYR A		79.770	3.566	10.090	1.00 15.70 A
	ATOM	600	OH	TYR A	146	80.999	3.473	9.491	1.00 16.29 A
	ATOM	601	С	TYR A	146	73.591	4.135	12.154	1.00 16.74 A
	ATOM	602	0	TYR A		73.004	3.050	12.132	1.00 17.63 A
	111 011	002	\sim	T T I \ \ \		, 5.001	3.030	14.17	1.00 1/.00 A

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	ATOM	603	N	PHE			73.198	5.158	12.901		15.90 A
	ATOM	604	CA	PHE	Α	147	72.012	5.041	13.745		17.10 A
	ATOM	605	СВ	PHE	Α	147	72.265	4.057	14.932	1.00	14.80 A
	ATOM	606	CG	PHE	Α	147	73.509	4.366	15.747	1.00	16.36 A
5	ATOM	607		PHE			73.526	5.427	16.657		15.38 A
5			CD2				74.701				16.83 A
	ATOM	608		PHE				3.663	15.514		
	ATOM	609		PHE			74.709	5.801	17.314		15.96 A
	MOTA	610	CE2	PHE	Α	147	75.907	4.024	16.163	1.00	16.65 A
	ATOM	611	CZ	PHE	Α	147	75.908	5.107	17.069	1.00	16.96 A
10	ATOM	612	С	PHE	Α	147	71.550	6.378	14.286	1.00	17.73 A
	ATOM	613	0	PHE			72.225	7.399	14.145		18.47 A
		614					70.376	6.352	14.897		19.28 A
	ATOM		N	THR							
	MOTA	615	CA	THR			69.801	7.529	15.532		19.50 A
	MOTA	616	СВ	THR	Α	148	68.846	8.308	14.597	1.00	19.24 A
15	ATOM	617	OG1	THR	Α	148	67.722	7.485	14.271	1.00	18.29 A
	MOTA	618	CG2	THR	Α	148	69.563	8.727	13.311	1.00	18.53 A
	ATOM	619	С	THR			68.976	7.071	16.718	1.00	19.68 A
	ATOM	620	0	THR			68.556	5.915	16.802		20.20 A
	ATOM	621	N	PHE			68.765	7.975	17.653		20.20 A
20	ATOM	622	CA	PHE			67.926	7.687	18.797		20.34 A
	MOTA	623	CB	PHE	Α	149	68.558	6.626	19.728	1.00	19.06 A
	ATOM	624	CG	PHE	Α	149	69.932	6.961	20.216	1.00	18.27 A
	ATOM	625	CD1	PHE	Δ	149	70.114	7.745	21.357		19.90 A
	ATOM	626		PHE			71.049	6.467	19.559		19.21 A
25											
25	ATOM	627	CE1	PHE			71.387	8.028	21.840		19.04 A
	ATOM	628	CE2	PHE	A	149	72.341	6.741	20.025		19.95 A
	MOTA	629	CZ	PHE	Α	149	72.513	7.520	21.167	1.00	21.19 A
	ATOM	630	С	PHE	Α	149	67.693	9.004	19.487	1.00	20.94 A
	ATOM	631	0	PHE	А	149	68.192	10.035	19.042	1.00	17.91 A
30	ATOM	632	N	GLN			66.888	8.988	20.539		25.44 A
30											
	ATOM	633	CA	GLN			66.609	10.212	21.279		29.09 A
	MOTA	634	СВ	GLN			65.518	11.039	20.571		29.07 A
	MOTA	635	CG	GLN	Α	150	64.194	10.322	20.309		31.07 A
	MOTA	636	CD	GLN	Α	150	63.150	11.227	19.609	1.00	32.52 A
35	ATOM	637	OE1	GLN	Α	150	62.503	12.075	20.243	1.00	30.50 A
	ATOM	638	NE2	GLN	Α	150	63.009	11.056	18.294	1.00	29.34 A
	ATOM	639	C	GLN			66.190	9.927	22.707		29.59 A
								8.832	23.018		
	ATOM	640	0	GLN			65.738				30.34 A
	ATOM	641	N	ASP			66.407	10.892	23.590		31.52 A
40	MOTA	642	CA	ASP			65.957	10.750	24.967		32.22 A
	MOTA	643	СВ	ASP	Α	151	67.093	10.948	25.974	1.00	31.30 A
	MOTA	644	CG	ASP	Α	151	67.832	12.246	25.790	1.00	32.39 A
	ATOM	645		ASP	Α	151	67.241	13.217	25.263	1.00	34.30 A
	ATOM	646		ASP			69.011	12.290	26.195		32.02 A
45				ASP							33.56 A
43	ATOM	647	С				64.914	11.858	25.063		
	MOTA	648	0	ASP			64.495	12.387	24.033		34.76 A
	ATOM	649	N	ASP	Α	152	64.498	12.239	26.261	1.00	35.00 A
	ATOM	650	CA	ASP	Α	152	63.462	13.268	26.369	1.00	36.72 A
	ATOM	651	СВ	ASP	Α	152	63.053	13.465	27.830	1.00	38.27 A
50	ATOM	652	CG	ASP			62.237	12.312	28.351		42.45 A
20	ATOM	653		ASP			61.377	11.824	27.579		43.52 A
	ATOM	654		ASP			62.444	11.900	29.519		44.28 A
	MOTA	655	С	ASP			63.758	14.627	25.759		36.47 A
	ATOM	656	0	ASP	Α	152	62.857	15.289	25.242	1.00	36.12 A
55	ATOM	657	N	GLU	Α	153	65.021	15.029	25.781	1.00	36.09 A
	ATOM	658	CA	GLU			65.358	16.343	25.292		35.16 A
	ATOM	659	CB	GLU			65.976	17.137	26.442		39.45 A
	ATOM	660	CG	GLU			65.486	16.714	27.830		45.94 A
	ATOM	661	CD	GLU	А	T22	66.383	15.652	28.468	1.00	51.78 A

	MOTA	662	OE1	GLU A	. 153	67.563	15.977	28.746	1.00 54.51 A
	MOTA	663	OE2	GLU A	. 153	65.924	14.500	28.689	1.00 52.47 A
	ATOM	664	С	GLU A		66.258	16.455	24.073	1.00 32.91 A
_	ATOM	665	0	GLU A		66.304	17.524	23.457	1.00 31.19 A
5	MOTA	666	N	LYS A		66.959	15.376	23.710	1.00 30.19 A
	ATOM	667	CA	LYS A	. 154	67.898	15.431	22.582	1.00 26.56 A
	ATOM	668	СВ	LYS A	154	69.323	15.414	23.121	1.00 24.92 A
	ATOM	669	CG	LYS A		69.630	16.551	24.041	1.00 23.66 A
	ATOM	670	CD	LYS A		70.944	16.355	24.750	1.00 20.95 A
10	ATOM	671	CE	LYS A	. 154	71.274	17.583	25.576	1.00 18.98 A
	MOTA	672	NZ	LYS A	. 154	72.491	17.388	26.360	1.00 19.19 A
	ATOM	673	С	LYS A	154	67.806	14.374	21.487	1.00 25.00 A
	ATOM	674	0	LYS A		67.342	13.257	21.701	1.00 25.62 A
	ATOM	675	N	LEU A		68.276	14.759	20.308	1.00 23.36 A
15	ATOM	676	CA	LEU A	. 155	68.337	13.881	19.140	1.00 22.19 A
	ATOM	677	СВ	LEU A	. 155	67.946	14.624	17.864	1.00 21.64 A
	ATOM	678	CG	LEU A	155	66.539	15.167	17.707	1.00 22.58 A
	ATOM	679		LEU A		66.437	15.847	16.350	1.00 22.74 A
	ATOM	680		LEU A		65.533	14.034	17.815	1.00 23.23 A
20	ATOM	681	С	LEU A	. 155	69.798	13.474	19.004	1.00 20.69 A
	ATOM	682	0	LEU A	. 155	70.693	14.287	19.249	1.00 21.61 A
	ATOM	683	N	TYR A	156	70.036	12.238	18.592	1.00 18.69 A
	ATOM	684	CA	TYR A		71.393	11.737	18.431	1.00 18.65 A
	ATOM	685	СВ	TYR A		71.690	10.661	19.489	1.00 18.51 A
25	MOTA	686	CG	TYR A	. 156	71.602	11.148	20.913	1.00 17.86 A
	ATOM	687	CD1	TYR A	. 156	70.372	11.287	21.550	1.00 18.38 A
	ATOM	688	CE1	TYR A	156	70.286	11.752	22.862	1.00 18.95 A
	ATOM	689	CD2	TYR A		72.755	11.488	21.621	1.00 19.32 A
• •	ATOM	690	CE2	TYR A		72.690	11.957	22.942	1.00 18.14 A
30	ATOM	691	CZ	TYR A	. 156	71.449	12.086	23.551	1.00 18.56 A
	ATOM	692	OH	TYR A	. 156	71.372	12.547	24.838	1.00 18.33 A
	ATOM	693	С	TYR A	156	71.640	11.125	17.059	1.00 18.03 A
	ATOM	694	0	TYR A		70.903	10.250	16.646	1.00 18.18 A
	ATOM	695	N	PHE A		72.662	11.568	16.338	1.00 17.19 A
35	ATOM	696	CA	PHE A	. 157	72.937	10.934	15.062	1.00 17.15 A
	ATOM	697	СВ	PHE A	. 157	72.980	11.951	13.918	1.00 21.54 A
	ATOM	698	CG	PHE A	157	71.663	12.638	13.651	1.00 26.82 A
	ATOM	699		PHE A		70.471	12.165	14.221	1.00 30.87 A
4.0	ATOM	700	CD2	PHE A		71.617	13.794	12.869	1.00 28.42 A
40	ATOM	701	CE1	PHE A		69.249	12.845	14.024	1.00 30.45 A
	MOTA	702	CE2	PHE A	. 157	70.407	14.483	12.661	1.00 29.44 A
	ATOM	703	CZ	PHE A	. 157	69.224	14.008	13.243	1.00 30.41 A
	ATOM	704	С	PHE A		74.286	10.244	15.184	1.00 16.38 A
	ATOM	705	0	PHE A		75.256	10.883	15.527	1.00 17.91 A
15									
45	ATOM	706	N	GLY A		74.347	8.942	14.919	1.00 16.20 A
	MOTA	707	CA	GLY A	. 158	75.614	8.232	15.009	1.00 15.78 A
	ATOM	708	С	GLY A	. 158	76.322	8.285	13.671	1.00 16.51 A
	ATOM	709	0	GLY A	158	75.876	7.659	12.710	1.00 17.95 A
	ATOM	710	N	LEU A		77.423	9.028	13.600	1.00 14.97 A
50									
50	ATOM	711	CA	LEU A		78.143	9.177	12.342	1.00 15.17 A
	MOTA	712	СВ	LEU A	. 159	78.264	10.669	12.012	1.00 13.14 A
	ATOM	713	CG	LEU A	. 159	76.989	11.518	12.133	1.00 12.95 A
	ATOM	714	CD1	LEU A		77.347	13.002	11.872	1.00 7.84 A
	ATOM	715		LEU A		75.926	11.020	11.138	1.00 11.24 A
55	ATOM	716	С	LEU A		79.535	8.540	12.300	1.00 15.49 A
	ATOM	717	0	LEU A	. 159	80.136	8.256	13.333	1.00 15.76 A
	ATOM	718	N	SER A	. 160	80.051	8.313	11.097	1.00 14.32 A
	ATOM	719	CA	SER A		81.389	7.759	10.984	1.00 14.68 A
			CB						
	ATOM	720	CD	SER A	. TOO	81.699	7.386	9.529	1.00 12.79 A

	7.03.6	701	0.6		1.60	01 205	0 100	0 606	1 00 16 15 7
	ATOM	721	OG	SER A		81.395	8.432	8.626	1.00 16.15 A
	ATOM	722	С	SER A	160	82.365	8.823	11.509	1.00 15.82 A
	ATOM	723	0	SER A	160	82.152	10.029	11.333	1.00 17.75 A
	ATOM	724	N	TYR A	161	83.418	8.386	12.184	1.00 16.30 A
5	ATOM	725	CA	TYR A		84.399	9.309	12.740	1.00 17.11 A
5						84.863			
	ATOM	726	СВ	TYR A			8.785	14.100	1.00 16.09 A
	MOTA	727	CG	TYR A	161	86.020	9.529	14.717	1.00 19.80 A
	MOTA	728	CD1	TYR A	161	86.070	10.933	14.700	1.00 18.64 A
	ATOM	729	CE1	TYR A	161	87.091	11.625	15.345	1.00 19.50 A
10	ATOM	730	CD2	TYR A	161	87.032	8.837	15.394	1.00 20.09 A
	ATOM	731	CE2	TYR A		88.057	9.517	16.047	1.00 21.66 A
	ATOM	732	CZ	TYR A		88.085	10.918	16.022	1.00 23.52 A
	ATOM	733	OH	TYR A		89.111	11.600	16.674	1.00 22.64 A
	MOTA	734	С	TYR A	161	85.594	9.495	11.815	1.00 17.86 A
15	ATOM	735	0	TYR A	161	86.269	8.527	11.459	1.00 19.30 A
	ATOM	736	N	ALA A		85.854	10.736	11.418	1.00 18.22 A
		737	CA	ALA A		86.990	11.040	10.546	1.00 19.59 A
	ATOM								
	ATOM	738	СВ	ALA A		86.569	12.063	9.466	1.00 19.99 A
	ATOM	739	С	ALA A	162	88.051	11.629	11.472	1.00 19.11 A
20	ATOM	740	0	ALA A	162	88.050	12.828	11.736	1.00 18.81 A
	ATOM	741	N	ALA A	163	88.952	10.775	11.956	1.00 18.78 A
	ATOM	742	CA	ALA A		89.994	11.165	12.918	1.00 18.84 A
	MOTA	743	СВ	ALA A		90.867	9.924	13.279	1.00 19.04 A
	ATOM	744	С	ALA A		90.908	12.357	12.604	1.00 18.22 A
25	MOTA	745	0	ALA A	163	91.290	13.101	13.508	1.00 16.79 A
	ATOM	746	N	ASN A	164	91.251	12.560	11.340	1.00 17.46 A
	ATOM	747	CA	ASN A	164	92.148	13.645	11.023	1.00 17.79 A
	ATOM	748	СВ	ASN A		92.990	13.270	9.803	1.00 20.45 A
• •	ATOM	749	CG	ASN A		93.919	12.092	10.097	1.00 21.08 A
30	ATOM	750		ASN A		94.663	12.117	11.066	1.00 21.57 A
	MOTA	751	ND2	ASN A	164	93.862	11.059	9.271	1.00 24.54 A
	ATOM	752	С	ASN A	164	91.555	15.044	10.889	1.00 18.34 A
	ATOM	753	0	ASN A		92.293	16.005	10.634	1.00 19.83 A
	ATOM	754	N	GLY A		90.247	15.176	11.083	1.00 15.01 A
25									
35	ATOM	755	CA	GLY A		89.644	16.490	11.022	1.00 15.54 A
	ATOM	756	С	GLY A	165	89.580	17.212	9.683	1.00 17.67 A
	MOTA	757	0	GLY A	165	89.607	16.600	8.613	1.00 19.49 A
	ATOM	758	N	GLU A	166	89.510	18.534	9.753	1.00 17.46 A
	ATOM	759	CA	GLU A	166	89.378	19.379	8.577	1.00 19.26 A
40	ATOM	760	СВ	GLU A		89.064	20.805	9.019	1.00 21.87 A
40									1.00 24.70 A
	ATOM	761	CG	GLU A		88.057	20.917	10.149	
	MOTA	762	CD	GLU A		87.723	22.359	10.477	1.00 26.05 A
	ATOM	763	OE1	GLU A	166	88.469	23.251	10.001	1.00 25.93 A
	ATOM	764	OE2	GLU A	166	86.726	22.598	11.213	1.00 25.24 A
45	ATOM	765	С	GLU A	166	90.538	19.441	7.592	1.00 20.11 A
	ATOM	766	0	GLU A		91.707	19.501	7.978	1.00 22.88 A
	ATOM	767	N	LEU A		90.195	19.443	6.312	1.00 18.72 A
	MOTA	768	CA	LEU A	167	91.173	19.565	5.242	1.00 17.38 A
	MOTA	769	СВ	LEU A	167	90.463	19.516	3.888	1.00 15.71 A
50	ATOM	770	CG	LEU A	167	91.238	19.817	2.601	1.00 15.42 A
	ATOM	771	CD1	LEU A		92.242	18.704	2.343	1.00 14.98 A
	ATOM	772		LEU A		90.265	19.947	1.416	1.00 12.32 A
	ATOM	773	С	LEU A		91.817	20.940	5.438	1.00 19.75 A
	ATOM	774	0	LEU A	167	93.030	21.103	5.266	1.00 19.61 A
55	ATOM	775	N	LEU A	168	91.001	21.928	5.812	1.00 20.53 A
	ATOM	776	CA	LEU A		91.516	23.277	6.033	1.00 22.20 A
	ATOM	777	СВ	LEU A		90.436	24.192	6.637	1.00 20.41 A
	ATOM	778	CG	LEU A		90.923	25.611	7.024	1.00 21.71 A
	ATOM	779	CDI	LEU A	т 68	91.275	26.413	5.768	1.00 20.09 A

	ATOM	780	CD2	LEU A	168	89.837	26.341	7.797		20.84 A
	MOTA	781	С	LEU A	168	92.731	23.245	6.968	1.00 2	23.07 A
	ATOM	782	0	LEU A	168	93.636	24.054	6.838	1.00 2	22.18 A
	ATOM	783	N	LYS A		92.742	22.305	7.905		24.67 A
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5	ATOM	784	CA	LYS A		93.844	22.192	8.850		28.56 A
	MOTA	785	CB	LYS A	169	93.561	21.076	9.858	1.00 3	31.12 A
	ATOM	786	CG	LYS A	169	94.615	20.933	10.938	1.00 3	85.60 A
	ATOM	787	CD	LYS A		94.436	19.652	11.765		39.37 A
	ATOM	788	CE	LYS A		94.832	18.410	10.961		12.26 A
10	MOTA	789	NZ	LYS A	169	94.664	17.131	11.725	1.00 4	12.83 A
	ATOM	790	С	LYS A	169	95.151	21.902	8.119	1.00 2	29.24 A
	ATOM	791	0	LYS A		96.190	22.505	8.398		30.32 A
	MOTA	792	N	TYR A		95.101	20.970	7.179		29.12 A
	MOTA	793	CA	TYR A	170	96.290	20.619	6.423	1.00 2	28.18 A
15	MOTA	794	СВ	TYR A	170	96.037	19.344	5.637	1.00 2	25.30 A
	ATOM	795	CG	TYR A	170	95.926	18.182	6.569		7.01 A
		796								
	ATOM			TYR A		97.072	17.533	7.053		26.92 A
	ATOM	797	CEI	TYR A	170	96.974	16.532	8.008		25.37 A
	ATOM	798	CD2	TYR A	170	94.688	17.792	7.062	1.00 2	25.14 A
20	ATOM	799	CE2	TYR A	170	94.580	16.807	8.009	1.00 2	26.49 A
	ATOM	800	CZ	TYR A		95.720	16.179	8.484		26.98 A
	MOTA	801	OH	TYR A		95.580	15.223	9.456		27.66 A
	MOTA	802	С	TYR A	170	96.690	21.742	5.507	1.00 2	28.69 A
	ATOM	803	0	TYR A	170	97.875	21.971	5.285	1.00 3	30.98 A
25	ATOM	804	N	ILE A	171	95.705	22.452	4.976	1.00 2	8.95 A
	ATOM	805	CA	ILE A		96.006	23.550	4.088		29.79 A
	MOTA	806	СВ	ILE A		94.721	24.233	3.579		29.29 A
	ATOM	807	CG2	ILE A	171	95.082	25.439	2.714	1.00 2	28.21 A
	MOTA	808	CG1	ILE A	171	93.906	23.227	2.747	1.00 2	9.66 A
30	ATOM	809	CD1	ILE A		92.567	23.754	2.224	1 00 2	9.13 A
50	ATOM	810	C	ILE A		96.897	24.536	4.833		31.13 A
	MOTA	811	0	ILE A		97.925	24.956	4.300		30.93 A
	MOTA	812	N	ARG A	172	96.525	24.862	6.075	1.00 3	32.00 A
	MOTA	813	CA	ARG A	172	97.294	25.789	6.903	1.00 3	32.60 A
35	ATOM	814	СВ	ARG A		96.527	26.175	8.163		32.77 A
55										
	ATOM	815	CG	ARG A		95.257	26.982	7.972		88.24 A
	ATOM	816	CD	ARG A		94.853	27.602	9.335		13.47 A
	MOTA	817	NE	ARG A	172	93.501	28.181	9.412	1.00 4	l6.65 A
	MOTA	818	CZ	ARG A	172	92.903	28.888	8.448	1.00 4	17.62 A
40	ATOM	819	NH1	ARG A		93.517	29.115	7.287	1.00 4	17.16 A
10		820		ARG A		91.691	29.398	8.659		15.61 A
	ATOM									
	ATOM	821	С	ARG A		98.646	25.219	7.338		32.95 A
	MOTA	822	0	ARG A	172	99.644	25.920	7.311	1.00 3	34.27 A
	MOTA	823	N	ALA A	173	98.674	23.960	7.761	1.00 3	32.74 A
45	ATOM	824	CA	ALA A		99.912	23.341	8.209		32.81 A
15										
	ATOM	825	СВ	ALA A		99.668	21.896	8.619		32.72 A
	ATOM	826	С	ALA A	173	101.005	23.400	7.152	1.00 3	33.67 A
	ATOM	827	0	ALA A	173	102.125	23.817	7.438	1.00 3	33.78 A
	ATOM	828	N	ILE A	174	100.698	22.995	5.926	1.00 3	3.50 A
50	ATOM	829	CA	ILE A		101.728	23.030	4.896		33.22 A
50										
	MOTA	830	СВ	ILE A		101.731	21.736	4.043		33.98 A
	MOTA	831	CG2	ILE A	174	101.725	20.502	4.950	1.00 3	32.94 A
	MOTA	832	CG1	ILE A	174	100.517	21.709	3.125	1.00 3	3.93 A
	ATOM	833		ILE A		100.602	20.631	2.080		36.79 A
55	ATOM	834	C	ILE A		101.638	24.231	3.957		32.69 A
55										
	MOTA	835	0	ILE A		102.326	24.269	2.938		33.88 A
	ATOM	836	N	GLY A	175	100.792	25.204	4.287	1.00 3	31.76 A
	ATOM	837	CA	GLY A	175	100.671	26.386	3.446	1.00 3	32.03 A
	ATOM	838	С	GLY A		99.838	26.223	2.184		32.77 A
	111 011	550	_	- L L L	/ 0	22.030	20.223	2.104	1.00	/ A

	MOTA	839	0	GLY	Α	175	98.870	26.958	1.976		35.12 A
	MOTA	840	N	SER	Α	176	100.225	25.291	1.322	1.00	31.63 A
	MOTA	841	CA	SER	Α	176	99.489	25.018	0.091	1.00	31.11 A
	MOTA	842	СВ	SER	Α	176	99.810	26.040	-0.996	1.00	31.54 A
5	ATOM	843	OG	SER	Α	176	101.141	25.874	-1.464	1.00	33.96 A
	ATOM	844	С	SER	Α	176	99.946	23.640	-0.354	1.00	30.72 A
	ATOM	845	0	SER	Α	176	100.977	23.154	0.111	1.00	31.29 A
	ATOM	846	N	PHE	Α	177	99.180	23.018	-1.246	1.00	28.27 A
	ATOM	847	CA	PHE	Α	177	99.475	21.683	-1.738	1.00	26.97 A
10	ATOM	848	СВ	PHE	Α	177	98.169	20.948	-2.060	1.00	27.18 A
	ATOM	849	CG	PHE	Α	177	97.376	20.530	-0.854	1.00	27.90 A
	ATOM	850	CD1	PHE	А	177	97.551	21.155	0.379	1.00	26.91 A
	ATOM	851	CD2	PHE			96.432	19.503	-0.957		27.62 A
	ATOM	852	CE1	PHE	А	177	96.812	20.762	1.477		26.03 A
15	ATOM	853	CE2	PHE			95.684	19.106	0.144		23.95 A
	ATOM	854	CZ	PHE			95.873	19.730	1.357		25.81 A
	ATOM	855	C	PHE			100.299	21.726	-3.008		26.99 A
	ATOM	856	0	PHE			100.115	22.618	-3.832		27.45 A
	ATOM	857	N	ASP			101.200	20.762	-3.179		26.09 A
20	ATOM	858	CA	ASP			101.260	20.704	-4.411		26.09 A
20	ATOM	859	CB	ASP			103.135	19.730	-4.303		27.73 A
	ATOM	860	CG	ASP			102.689	18.318	-4.023		33.79 A
	ATOM	861		ASP			101.601	17.919	-4.510		37.57 A
	ATOM	862		ASP			103.431	17.590	-3.324		35.89 A
25	ATOM	863	C	ASP			100.955	20.202	-5.443		25.72 A
23	ATOM	864	0	ASP			99.763	20.202	-5.128		24.80 A
	ATOM	865	N	GLU			101.419	19.897	-6.650		24.80 A
		866	CA	GLU			100.514	19.444	-7.697		25.67 A
	ATOM			GLU			101.187	19.554			27.44 A
30	ATOM	867	CB CG	GLU			100.197		-9.052 -10.129		31.17 A
30	ATOM	868	CD						-10.129		35.24 A
	ATOM	869		GLU			100.823				
	ATOM	870		GLU			102.016		-11.572		35.82 A
	ATOM	871	OE2	GLU			100.116		-12.488		38.12 A
25	ATOM	872	C	GLU			99.917	18.041	-7.560		24.90 A
35	ATOM	873	0	GLU			98.755	17.822	-7.894		23.01 A
	ATOM	874	N	THR			100.709	17.095	-7.082		24.57 A
	ATOM	875	CA	THR			100.240	15.723	-6.923		25.53 A
	ATOM	876	CB	THR			101.395	14.803	-6.478		24.65 A
40	ATOM	877		THR			102.525	15.069	-7.304		25.84 A
40	ATOM	878	CG2	THR			101.021	13.334	-6.624		23.39 A
	ATOM	879	С	THR			99.110	15.623	-5.902		25.85 A
	ATOM	880	0	THR			98.149	14.892	-6.111		25.59 A
	ATOM	881	N	CYS			99.237	16.359	-4.799		25.83 A
45	ATOM	882	CA	CYS			98.217	16.355	-3.752		26.26 A
45	ATOM	883	СВ	CYS			98.778	16.939	-2.451		27.81 A
	ATOM	884	SG	CYS			100.202	16.031	-1.775		32.72 A
	ATOM	885	С	CYS			96.963	17.127	-4.169		25.20 A
	ATOM	886	0	CYS			95.853	16.696	-3.878		26.19 A
50	ATOM	887	N	THR			97.139	18.262	-4.841		22.74 A
50	ATOM	888	CA	THR			96.002	19.046	-5.305		21.82 A
	ATOM	889	CB	THR			96.453	20.308	-6.103		21.81 A
	ATOM	890		THR			97.258	21.161	-5.276		24.55 A
	ATOM	891		THR			95.252	21.080	-6.593		18.62 A
	ATOM	892	С	THR			95.197	18.141	-6.249		23.45 A
55	ATOM	893	0	THR			93.975	17.997	-6.116		22.94 A
	ATOM	894	N	ARG			95.897	17.528	-7.202		22.71 A
	ATOM	895	CA	ARG			95.260	16.648	-8.158		23.26 A
	ATOM	896	СВ	ARG			96.285	16.118	-9.171		22.46 A
	ATOM	897	CG	ARG	Α	183	95.692	15.140	-10.184	1.00	24.96 A

	ATOM	898	CD	ARG A	183	96.762	14.512	-11.078	1.00 27.09 A
	MOTA	899	NE	ARG A	183	97.372	15.577	-11.849	1.00 33.02 A
	ATOM	900	CZ	ARG A	183	98.637	15.948	-11.732	1.00 33.62 A
	ATOM	901	NH1	ARG A	183	99.440	15.312	-10.885	1.00 32.57 A
5	ATOM	902		ARG A		99.069		-12.404	1.00 33.25 A
J		903				94.559	15.475	-7.459	
	ATOM		C	ARG A					1.00 22.42 A
	ATOM	904	0	ARG A		93.393	15.193	-7.721	1.00 21.37 A
	ATOM	905	N	PHE A		95.255	14.800	-6.562	1.00 21.19 A
	ATOM	906	CA	PHE A	184	94.630	13.673	-5.888	1.00 22.20 A
10	MOTA	907	СВ	PHE A	184	95.615	12.964	-4.966	1.00 23.58 A
	ATOM	908	CG	PHE A	184	95.029	11.766	-4.283	1.00 25.43 A
	ATOM	909	CD1	PHE A	184	94.916	10.556	-4.954	1.00 25.01 A
	ATOM	910	CD2	PHE A		94.508	11.867	-2.998	1.00 24.35 A
	ATOM	911		PHE A		94.285	9.460	-4.356	1.00 23.50 A
15	ATOM	912	CE2	PHE A		93.881	10.782	-2.409	1.00 24.71 A
13									
	ATOM	913	CZ	PHE A		93.771	9.577	-3.094	1.00 22.95 A
	ATOM	914	С	PHE A		93.405	14.074	-5.072	1.00 21.96 A
	ATOM	915	0	PHE A		92.348	13.450	-5.170	1.00 21.31 A
	ATOM	916	N	TYR A	185	93.544	15.116	-4.267	1.00 21.18 A
20	MOTA	917	CA	TYR A	185	92.433	15.543	-3.445	1.00 20.50 A
	ATOM	918	СВ	TYR A	185	92.956	16.425	-2.313	1.00 21.33 A
	ATOM	919	CG	TYR A	185	93.494	15.550	-1.190	1.00 22.24 A
	ATOM	920	CD1	TYR A		92.641	14.670	-0.507	1.00 21.55 A
	ATOM	921	CE1	TYR A		93.127	13.755	0.414	1.00 20.71 A
25	ATOM	922	CD2	TYR A		94.853	15.497	-0.904	1.00 20.71 A
23		923	CE2						1.00 21.37 A
	ATOM			TYR A		95.353	14.579	0.019	
	ATOM	924	CZ	TYR A		94.486	13.705	0.670	1.00 21.18 A
	ATOM	925	OH	TYR A		94.986	12.746	1.519	1.00 19.84 A
	MOTA	926	С	TYR A		91.273	16.182	-4.201	1.00 19.27 A
30	ATOM	927	0	TYR A	185	90.112	16.056	-3.801	1.00 17.72 A
	MOTA	928	N	THR A	186	91.576	16.834	-5.314	1.00 17.25 A
	ATOM	929	CA	THR A	186	90.527	17.433	-6.110	1.00 15.61 A
	ATOM	930	СВ	THR A	186	91.097	18.366	-7.188	1.00 15.69 A
	ATOM	931	OG1	THR A		91.710	19.508	-6.564	1.00 16.11 A
35	ATOM	932	CG2	THR A		89.996	18.816	-8.135	1.00 12.68 A
55	ATOM	933	C	THR A		89.756	16.302	-6.785	1.00 15.75 A
			0					-6.899	1.00 15.75 A
	ATOM	934		THR A		88.523	16.350		
	ATOM	935	N	ALA A		90.478	15.277	-7.218	1.00 14.94 A
4.0	ATOM	936	CA	ALA A		89.841	14.136	-7.868	1.00 16.15 A
40	ATOM	937	СВ	ALA A		90.905	13.130	-8.382	1.00 13.30 A
	MOTA	938	С	ALA A		88.847	13.450	-6.911	1.00 16.71 A
	MOTA	939	0	ALA A	187	87.743	13.075	-7.328	1.00 16.50 A
	MOTA	940	N	GLU A	188	89.213	13.308	-5.635	1.00 17.10 A
	MOTA	941	CA	GLU A	188	88.302	12.673	-4.679	1.00 17.85 A
45	ATOM	942	СВ	GLU A		88.953	12.514	-3.302	1.00 18.83 A
	ATOM	943	CG	GLU A		90.219	11.665	-3.296	1.00 19.46 A
	ATOM	944	CD	GLU A		90.370	10.795	-2.050	1.00 20.84 A
	ATOM	945		GLU A		90.131	11.276	-0.920	1.00 20.01 A
50	ATOM	946		GLU A			9.616	-2.207	1.00 23.35 A
50	ATOM	947	С	GLU A		87.043	13.516	-4.551	1.00 17.79 A
	ATOM	948	0	GLU A		85.921	13.005	-4.579	1.00 18.83 A
	ATOM	949	N	ILE A	189	87.220	14.824	-4.449	1.00 17.09 A
	ATOM	950	CA	ILE A	189	86.060	15.688	-4.312	1.00 15.61 A
	ATOM	951	СВ	ILE A	189	86.495	17.141	-4.054	1.00 15.83 A
55	ATOM	952	CG2	ILE A		85.278	18.019	-3.853	1.00 14.16 A
	ATOM	953		ILE A		87.380	17.199	-2.794	1.00 17.34 A
	ATOM	954		ILE A		87.949	18.583	-2.479	1.00 15.37 A
	ATOM	955	C	ILE A		85.176	15.611	-5.558	1.00 15.37 A
		956	0						1.00 15.00 A
	ATOM	900	U	ILE A	103	83.953	15.530	-5.460	1.00 13.32 A

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	ATOM	957	N	VAL	Α	190	85.794	15.619	-6.733		15.46 A	
	ATOM	958	CA	VAL	Α	190	85.031	15.570	-7.964	1.00	15.38 A	r
	ATOM	959	СВ	VAL	Α	190	85.975	15.641	-9.181	1.00	15.37 A	١
	ATOM	960		VAL			85.273		-10.447		14.43 A	
_												
5	MOTA	961		VAL			86.454	17.056	-9.350		14.03 A	
	ATOM	962	С	VAL	Α	190	84.228	14.279	-7.987	1.00	17.35 A	L
	ATOM	963	0	VAL	Α	190	83.016	14.281	-8.258	1.00	15.96 A	r
	ATOM	964	N	SER	Α	191	84.916	13.182	-7.683	1.00	17.90 A	
		965	CA	SER			84.305	11.858	-7.660		17.77 A	
1.0	ATOM											
10	MOTA	966	СВ	SER			85.377	10.811	-7.344		18.25 A	
	ATOM	967	OG	SER	Α	191	84.801	9.523	-7.243	1.00	21.13 A	L
	ATOM	968	С	SER	Α	191	83.147	11.778	-6.640	1.00	17.28 A	r
	ATOM	969	0	SER	Α	191	82.153	11.095	-6.865	1.00	15.44 A	
	ATOM	970	N	ALA			83.291	12.490	-5.525		17.27 A	
1.5												
15	MOTA	971	CA	ALA			82.267	12.529	-4.485		15.98 A	
	ATOM	972	СВ	ALA	Α	192	82.834	13.164	-3.191	1.00	14.89 A	r
	ATOM	973	С	ALA	Α	192	81.078	13.336	-4.988	1.00	16.44 A	r
	ATOM	974	0	ALA	Α	192	79.934	12.922	-4.816	1.00	17.59 A	
	ATOM	975	N	LEU			81.340	14.487	-5.609		16.63 A	
20												
20	MOTA	976	CA	LEU			80.253	15.303	-6.140		16.11 A	
	ATOM	977	СВ	LEU	Α	193	80.769	16.632	-6.688	1.00	16.40 A	r
	ATOM	978	CG	LEU	Α	193	81.421	17.545	-5.645	1.00	18.83 A	7
	ATOM	979	CD1	LEU	Α	193	81.779	18.885	-6.276	1.00	18.24 A	
	ATOM	980		LEU			80.455	17.751	-4.479		18.63 A	
25											16.95 A	
25	ATOM	981	С	LEU			79.509	14.551	-7.236			
	MOTA	982	0	LEU			78.286	14.623	-7.325		18.76 A	
	ATOM	983	N	GLU	Α	194	80.229	13.825	-8.079	1.00	17.87 A	r
	ATOM	984	CA	GLU	Α	194	79.539	13.082	-9.124	1.00	19.66 A	r
	ATOM	985	СВ	GLU	Δ	194	80.525	12.295	-9.990	1.00	21.82 A	
30		986	CG				79.844		-10.947		21.12 A	
30	ATOM			GLU								
	MOTA	987	CD	GLU			80.831		-11.758		25.70 A	
	ATOM	988	OE 1	GLU	Α	194	81.900	10.122	-11.216	1.00	27.41 A	r
	ATOM	989	OE2	GLU	Α	194	80.527	10.244	-12.939	1.00	26.12 A	7
	ATOM	990	С	GLU	Α	194	78.546	12.123	-8.479	1.00	19.58 A	
35	ATOM	991	0	GLU			77.420	11.987	-8.937		17.78 A	
33												
	MOTA	992	N	TYR			78.962	11.462	-7.406		19.09 A	
	ATOM	993	CA	TYR			78.063	10.545	-6.736		19.86 A	
	ATOM	994	СВ	TYR	Α	195	78.807	9.740	-5.673	1.00	20.01 A	r
	ATOM	995	CG	TYR	Α	195	77.871	8.975	-4.756	1.00	20.45 A	ı
40	MOTA	996	CD1	TYR			77.329	7.748	-5.142		19.40 A	
10	ATOM	997	CE1				76.471	7.044	-4.296		18.43 A	
	MOTA	998	CD2	TYR			77.527	9.482	-3.500		20.11 A	
	ATOM	999	CE2	TYR	Α	195	76.678	8.792	-2.652	1.00	19.96 A	r
	ATOM	1000	CZ	TYR	Α	195	76.154	7.567	-3.057	1.00	21.07 A	r
45	ATOM	1001	OH	TYR			75.336	6.859	-2.206	1.00	21.31 A	
	ATOM	1002	С	TYR			76.914	11.295	-6.060		20.00 A	
	ATOM	1003	0	TYR			75.775	10.823	-6.033		21.42 A	
	ATOM	1004	Ν	LEU	Α	196	77.222	12.455	-5.500	1.00	17.38 A	r
	ATOM	1005	CA	LEU	Α	196	76.209	13.226	-4.795	1.00	18.74 A	r
50	ATOM	1006	СВ	LEU	Α	196	76.846	14.412	-4.049	1.00	17.38 A	
	ATOM	1007	CG	LEU			75.850	15.100	-3.110		19.04 A	
	MOTA	1008		LEU			75.423	14.093	-2.061		17.66 A	
	ATOM	1009	CD2	LEU	Α	196	76.462	16.338	-2.453	1.00	19.54 A	L
	ATOM	1010	С	LEU	Α	196	75.148	13.747	-5.751	1.00	18.47 A	r
55	ATOM	1011	0	LEU			73.944	13.608	-5.523		15.05 A	
	ATOM	1012	N	HIS			75.622	14.361	-6.824		18.35 A	
	MOTA	1013	CA	HIS			74.740	14.915	-7.812		20.04 A	
	MOTA	1014	СВ	HIS	Α	197	75.562	15.809	-8.718		20.29 A	
	ATOM	1015	CG	HIS	Α	197	76.048	17.044	-8.025	1.00	21.90 A	r

		4046			_	4.00		45 500	6 504	4 00	40 40 -
	MOTA	1016		HIS			75.766	17.539	-6.794		19.49 A
	MOTA	1017		HIS			76.892	17.956	-8.621	1.00	20.69 A
	ATOM	1018	CE1	HIS	Α	197	77.104	18.960	-7.789	1.00	20.86 A
	ATOM	1019	NE2	HIS	Α	197	76.433	18.732	-6.676	1.00	19.12 A
5	ATOM	1020	С	HIS			73.950	13.858	-8.587		21.27 A
5	ATOM	1021	0	HIS			72.865	14.133	-9.099		21.27 A
	ATOM	1022	N	GLY			74.487	12.644	-8.644		21.36 A
	ATOM	1023	CA	GLY			73.810	11.569	-9.339		20.60 A
	ATOM	1024	С	GLY	Α	198	72.528	11.203	-8.632		22.72 A
10	MOTA	1025	0	GLY	Α	198	71.593	10.742	-9.269	1.00	22.75 A
	ATOM	1026	N	LYS	Α	199	72.478	11.411	-7.313	1.00	24.27 A
	ATOM	1027	CA	LYS	Α	199	71.280	11.105	-6.523	1.00	22.95 A
	ATOM	1028	СВ	LYS	Α	199	71.659	10.629	-5.123	1.00	24.67 A
	ATOM	1029	CG	LYS			72.570	9.429	-5.109		29.22 A
15	ATOM	1030	CD	LYS			72.986	9.064	-3.701		33.11 A
13											
	ATOM	1031	CE	LYS			72.531	7.660	-3.366		37.28 A
	ATOM	1032	NZ	LYS			72.917	6.686	-4.455		38.82 A
	ATOM	1033	С	LYS			70.432	12.354	-6.398		22.39 A
	ATOM	1034	0	LYS	Α	199	69.558	12.431	-5.542	1.00	22.53 A
20	MOTA	1035	N	GLY	Α	200	70.710	13.343	-7.241	1.00	21.56 A
	ATOM	1036	CA	GLY	Α	200	69.953	14.580	-7.203	1.00	22.28 A
	ATOM	1037	С	GLY			70.006	15.326	-5.882		23.53 A
	ATOM	1038	0	GLY			69.017	15.930	-5.461		24.83 A
	ATOM	1039	N	ILE			71.161	15.302	-5.225		22.74 A
25	ATOM	1040	CA	ILE			71.314	15.985	-3.951		22.74 A
23											
	ATOM	1041	CB	ILE			71.796	15.007	-2.842		22.51 A
	ATOM	1042	CG2	ILE			71.995	15.757	-1.536		21.73 A
	ATOM	1043	CG1	ILE			70.788	13.876	-2.638		22.48 A
	ATOM	1044	CD1	ILE	Α	201	71.274	12.791	-1.687	1.00	17.26 A
30	MOTA	1045	С	ILE	Α	201	72.361	17.086	-4.076	1.00	24.41 A
	MOTA	1046	0	ILE	Α	201	73.387	16.904	-4.737	1.00	26.41 A
	ATOM	1047	N	ILE	Α	202	72.118	18.236	-3.470	1.00	23.00 A
	ATOM	1048	CA	ILE			73.137	19.267	-3.520		24.60 A
	ATOM	1049	СВ	ILE			72.729	20.440	-4.420		26.37 A
35	ATOM	1050	CG2	ILE			72.503	19.934	-5.829		28.52 A
33		1050									
	ATOM		CG1	ILE			71.450	21.086	-3.922		29.04 A
	ATOM	1052	CD1	ILE			70.958	22.165	-4.845		32.55 A
	ATOM	1053	С	ILE			73.482	19.732	-2.105		24.36 A
	MOTA	1054	0	ILE			72.605	19.919	-1.257		25.89 A
40	MOTA	1055	N	HIS	Α	203	74.776	19.882	-1.856	1.00	22.94 A
	MOTA	1056	CA	HIS	Α	203	75.289	20.273	-0.555	1.00	22.27 A
	MOTA	1057	СВ	HIS	Α	203	76.800	20.010	-0.526	1.00	20.00 A
	ATOM	1058	CG	HIS	Α	203	77.401	20.051	0.840	1.00	18.45 A
	ATOM	1059	CD2	HIS	Α	203	77.865	19.060	1.640		19.77 A
45	ATOM	1060		HIS			77.569	21.222	1.542		16.33 A
15	ATOM	1061		HIS			78.115	20.953	2.715		17.77 A
	ATOM	1062		HIS			78.306	19.650	2.800		18.48 A
	MOTA	1063	С	HIS			74.978	21.731	-0.206		23.37 A
	ATOM	1064	0	HIS			74.411	22.009	0.860		22.52 A
50	ATOM	1065	N	ARG	Α	204	75.361	22.648	-1.101	1.00	23.22 A
	MOTA	1066	CA	ARG	Α	204	75.126	24.087	-0.934	1.00	23.42 A
	ATOM	1067	СВ	ARG	Α	204	73.674	24.375	-0.544	1.00	22.74 A
	ATOM	1068	CG	ARG	Α	204	72.663	23.966	-1.561	1.00	24.57 A
	ATOM	1069	CD	ARG			71.341	24.681	-1.325		26.51 A
55	ATOM	1070	NE	ARG			70.699	24.299	-0.074		28.25 A
55			CZ	ARG							28.63 A
	ATOM	1071					69.596	24.871	0.405		
	ATOM	1072		ARG			69.013	25.849	-0.267		28.47 A
	ATOM	1073		ARG			69.086	24.472	1.563		28.55 A
	ATOM	1074	С	ARG	Α	204	76.017	24.819	0.061	1.00	24.12 A

	7.001	1075	_		_	0.0.4	75 005	0.6.001	0 200	1 00	06 06 :	_
	ATOM	1075	0	ARG			75.805	26.001	0.308		26.26	
	MOTA	1076	N	ASP	Α	205	76.990	24.135	0.654	1.00	23.05	A
	ATOM	1077	CA	ASP	Α	205	77.887	24.789	1.595	1.00	20.96	Α
	ATOM	1078	СВ	ASP	Α	205	77.219	24.883	2.964	1.00	22.31 7	Α
5	ATOM	1079	CG	ASP			77.964	25.801	3.914		26.08 7	
5		1080		ASP					3.439		25.93	
	ATOM						78.812	26.582				
	ATOM	1081		ASP			77.707	25.751	5.141		29.89	
	ATOM	1082	С	ASP	Α	205	79.210	24.020	1.662	1.00	20.46	A
	ATOM	1083	0	ASP	Α	205	79.812	23.833	2.716	1.00	21.36	Α
10	ATOM	1084	N	LEU	Α	206	79.666	23.584	0.504	1.00	18.98 7	Α
	ATOM	1085	CA	LEU			80.893	22.827	0.407		19.83	
		1086	CB	LEU			80.983	22.229	-0.994		21.73	
	ATOM											
	ATOM	1087	CG	LEU			82.039	21.167	-1.298		24.76	
	ATOM	1088	CD1	LEU	Α	206	81.818	19.943	-0.401	1.00	24.95	A
15	MOTA	1089	CD2	LEU	Α	206	81.941	20.789	-2.778	1.00	23.74	Α
	MOTA	1090	С	LEU	Α	206	82.093	23.725	0.691	1.00	20.17	Α
	ATOM	1091	0	LEU			82.162	24.857	0.200	1.00	20.92	Δ
	ATOM	1092	N	LYS			83.044	23.226	1.475		19.79	
20	ATOM	1093	CA	LYS			84.233	24.004	1.821		19.45	
20	ATOM	1094	СВ	LYS			83.825	25.209	2.667		17.84	
	MOTA	1095	CG	LYS	Α	207	83.123	24.820	3.933	1.00	19.19 7	Α
	ATOM	1096	CD	LYS	Α	207	82.331	25.969	4.500	1.00	20.50 7	Α
	ATOM	1097	CE	LYS	А	207	81.663	25.556	5.797	1.00	22.10 2	А
	ATOM	1098	ΝZ	LYS			80.955	26.674	6.480		22.34	
25	ATOM	1099	C	LYS			85.241	23.130	2.565		19.59	
23												
	ATOM	1100	0	LYS			84.917	22.025	2.985		20.21	
	ATOM	1101	N	PRO			86.480	23.618	2.737		19.79	
	ATOM	1102	CD	PRO	Α	208	87.032	24.869	2.188	1.00	18.04 I	A
	MOTA	1103	CA	PRO	Α	208	87.526	22.853	3.428	1.00	19.22	Α
30	ATOM	1104	CB	PRO	Α	208	88.756	23.763	3.297	1.00	19.27	Α
	ATOM	1105	CG	PRO	Α	208	88.496	24.521	2.027	1.00	16.27	A
	ATOM	1106	С	PRO			87.221	22.477	4.883		20.50 7	
	ATOM	1107	0	PRO			87.791	21.511	5.411		21.44	
	ATOM	1108		GLU			86.335	23.231	5.530		20.19	
25			N									
35	ATOM	1109	CA	GLU			85.956	22.976	6.927		21.25	
	ATOM	1110	СВ	GLU			85.383	24.251	7.562		21.43	
	MOTA	1111	CG	GLU	Α	209	86.330	25.446	7.535	1.00	26.33 <i>I</i>	Α
	ATOM	1112	CD	GLU	Α	209	86.203	26.315	6.270	1.00	30.17	Α
	ATOM	1113	OE1	GLU	Α	209	86.143	25.785	5.131	1.00	30.44	Α
40	ATOM	1114		GLU			86.173	27.557	6.422		33.49	
.0	ATOM	1115	C	GLU			84.920	21.839	7.040		22.45	
	ATOM	1116	0	GLU			84.733	21.255	8.114		21.98	
	ATOM	1117	N	ASN			84.269	21.545	5.915		22.73	
	ATOM	1118	CA	ASN			83.234	20.514	5.788		23.66	
45	MOTA	1119	СВ	ASN	Α	210	82.102	21.013	4.882	1.00	26.67 <i>I</i>	Α
	ATOM	1120	CG	ASN	Α	210	81.104	21.881	5.613	1.00	33.39 7	Α
	ATOM	1121	OD1	ASN	Δ	210	80.223	22.481	4.988		36.52	
	ATOM	1122		ASN			81.221	21.950	6.946		34.23	
		1123						19.239				
50	ATOM		C	ASN			83.775		5.162		21.41	
50	ATOM	1124	0	ASN			83.067	18.244	5.081		21.16	
	ATOM	1125	N	ILE	Α	211	85.006	19.293	4.674		19.42	
	MOTA	1126	CA	ILE	Α	211	85.619	18.141	4.029	1.00	17.43	Α
	ATOM	1127	СВ	ILE	Α	211	86.319	18.556	2.708	1.00	14.89 7	A
	ATOM	1128		ILE			87.046	17.349	2.096		12.68	
55	ATOM	1129		ILE			85.277	19.157	1.736		13.30	
55												
	ATOM	1130		ILE			85.855	19.805	0.435		10.47	
	ATOM	1131	C	ILE			86.620	17.578	5.024		17.83	
	ATOM	1132	0	ILE			87.685	18.151	5.241		17.76	
	ATOM	1133	N	LEU	Α	212	86.265	16.457	5.639	1.00	16.05	Α

		4404			_	0.4.0	00 404	4 5 0 5 4		4 00	45.04	_
	ATOM	1134	CA	LEU			87.121	15.871	6.656		15.84	
	MOTA	1135	СВ	LEU	Α	212	86.256	15.319	7.793	1.00	14.28	Α
	ATOM	1136	CG	LEU	Α	212	85.108	16.227	8.285	1.00	14.68	Α
	ATOM	1137	CD1	LEU			84.606	15.715	9.647		11.38	
5	ATOM	1138	CD2	LEU			85.579	17.685	8.422		10.88	
)												
	ATOM	1139	С	LEU			88.031	14.787	6.114		16.77	
	ATOM	1140	0	LEU	Α	212	87.861	14.335	4.984	1.00	16.78	Α
	MOTA	1141	N	LEU	Α	213	88.999	14.374	6.925	1.00	16.47	Α
	ATOM	1142	CA	LEU	Α	213	89.924	13.332	6.516	1.00	17.64	Α
10	ATOM	1143	СВ	LEU			91.323	13.926	6.378		18.08	
10		1144									17.92	
	ATOM		CG	LEU			91.367	14.880	5.176			
	ATOM	1145		LEU			92.076	16.134	5.529		18.78	
	MOTA	1146	CD2	LEU	Α	213	92.042	14.187	4.000	1.00	17.07	Α
	ATOM	1147	С	LEU	Α	213	89.919	12.147	7.473	1.00	18.68	Α
15	ATOM	1148	0	LEU	Α	213	90.091	12.297	8.672	1.00	18.75	Α
	ATOM	1149	N	ASN			89.712	10.955	6.939		21.19	
	ATOM	1150	CA	ASN			89.673	9.780	7.797		23.68	
	ATOM	1151	СВ	ASN			88.864	8.657	7.122		25.68	
	MOTA	1152	CG	ASN	Α	214	89.613	7.979	6.012	1.00	31.70	Α
20	ATOM	1153	OD1	ASN	Α	214	90.680	8.426	5.590	1.00	35.54	Α
	ATOM	1154	ND2	ASN	Α	214	89.057	6.886	5.521	1.00	34.56	Α
	ATOM	1155	C	ASN			91.077	9.328	8.203		22.08	
	ATOM	1156	0	ASN			92.056	9.972	7.864		20.25	
	ATOM	1157	N	ALA			91.170	8.239	8.953		24.03	
25	ATOM	1158	CA	ALA	Α	215	92.464	7.738	9.420	1.00	24.26	Α
	ATOM	1159	CB	ALA	Α	215	92.276	6.502	10.277	1.00	21.70	Α
	ATOM	1160	С	ALA	Α	215	93.421	7.426	8.296	1.00	24.90	Α
	ATOM	1161	0	ALA			94.615	7.435	8.491		26.03	
		1162		ASP			92.889	7.143	7.108		25.93	
20	ATOM		N									
30	ATOM	1163	CA	ASP			93.726	6.826	5.963		26.29	
	ATOM	1164	СВ	ASP	Α	216	93.048	5.773	5.091	1.00	32.31	Α
	ATOM	1165	CG	ASP	Α	216	92.862	4.456	5.812	1.00	38.06	Α
	MOTA	1166	OD1	ASP	Α	216	93.780	4.043	6.559	1.00	40.03	Α
	ATOM	1167		ASP			91.800	3.823	5.616		42.79	
35	ATOM	1168	C	ASP			94.046	8.026	5.095		23.69	
33												
	ATOM	1169	0	ASP			94.717	7.899	4.085		24.38	
	ATOM	1170	N	MET			93.546	9.187	5.478		21.45	
	ATOM	1171	$^{\rm CA}$	MET			93.752	10.418	4.726	1.00	20.48	Α
	ATOM	1172	CB	MET	Α	217	95.226	10.614	4.396	1.00	21.48	Α
40	ATOM	1173	CG	MET	Α	217	96.081	10.894	5.629	1.00	21.46	Α
	ATOM	1174	SD	MET	Δ	217	95.504	12.311	6.580		25.32	
	ATOM	1175	CE	MET			96.079	13.722	5.573		24.08	
	ATOM								3.458			
		1176	С	MET			92.900	10.556			19.63	
	ATOM	1177	0	MET			93.245	11.294	2.546		19.54	
45	ATOM	1178	N	HIS			91.794	9.824	3.405	1.00	18.82	Α
	ATOM	1179	CA	HIS	Α	218	90.843	9.945	2.311	1.00	18.81	Α
	ATOM	1180	СВ	HIS	Α	218	90.206	8.589	1.994	1.00	20.61	Α
	ATOM	1181	CG	HIS			91.097	7.666	1.218		22.68	
							91.840	6.605			20.37	
50	ATOM	1182		HIS					1.614			
50	ATOM	1183		HIS			91.316	7.806	-0.139		21.30	
	ATOM	1184		HIS			92.153	6.867	-0.541	1.00	20.75	Α
	ATOM	1185	NE2	HIS	Α	218	92.485	6.128	0.501	1.00	20.31	Α
	ATOM	1186	С	HIS	Α	218	89.774	10.925	2.863	1.00	18.97	Α
	ATOM	1187	0	HIS			89.534	10.965	4.083		16.48	
55											17.41	
55	ATOM	1188	N	ILE			89.166	11.721	1.978			
	ATOM	1189	CA	ILE			88.165	12.702	2.387		16.48	
	ATOM	1190	СВ	ILE			87.765	13.695	1.242		13.43	
	ATOM	1191	CG2	ILE	Α	219	88.984	14.404	0.698	1.00	10.66	Α
	MOTA	1192	CG1	ILE	Α	219	86.973	12.952	0.156	1.00	11.14	Α

	ATOM	1193	CD1	ILE	Α	219	86.505	13.807	-0.995	1.00	4.26 A
	ATOM	1194	С	ILE	Α	219	86.875	12.067	2.864	1.00	17.14 A
	ATOM	1195	0	ILE	Α	219	86.541	10.943	2.497	1.00	18.77 A
	ATOM	1196	N	GLN			86.159	12.808	3.696		17.24 A
5	ATOM	1197	CA	GLN			84.878	12.376	4.203		18.93 A
)											
	ATOM	1198	СВ	GLN			85.002	11.756	5.604		22.02 A
	ATOM	1199	CG	GLN	Α	220	83.791	10.874	5.952	1.00	26.68 A
	ATOM	1200	CD	GLN	Α	220	83.949	10.071	7.253	1.00	31.76 A
	ATOM	1201	OE1	GLN	Α	220	83.437	10.471	8.331	1.00	27.57 A
10	ATOM	1202		GLN			84.667	8.930	7.161	1.00	29.97 A
	ATOM	1203	C	GLN			84.077	13.652	4.261		17.44 A
	ATOM	1204	0	GLN			84.247	14.465	5.170		17.81 A
	MOTA	1205	N	ILE			83.229	13.852	3.263		15.69 A
	MOTA	1206	CA	ILE	Α	221	82.413	15.051	3.230	1.00	16.08 A
15	MOTA	1207	СВ	ILE	Α	221	81.939	15.359	1.802	1.00	15.82 A
	ATOM	1208	CG2	ILE	Α	221	80.956	16.519	1.834	1.00	13.95 A
	ATOM	1209	CG1	ILE			83.163	15.627	0.899		16.66 A
	ATOM	1210	CD1	ILE			82.837	16.045	-0.548		13.13 A
	ATOM	1211	С	ILE			81.207	14.892	4.156		16.52 A
20	ATOM	1212	0	ILE	Α	221	80.542	13.860	4.157	1.00	16.03 A
	MOTA	1213	N	THR	Α	222	80.927	15.922	4.948	1.00	17.66 A
	MOTA	1214	CA	THR	Α	222	79.810	15.862	5.882	1.00	17.70 A
	ATOM	1215	СВ	THR	Α	222	80.331	15.433	7.277	1.00	18.71 A
	ATOM	1216		THR			79.230	15.263	8.172		16.76 A
25	ATOM	1217	CG2	THR			81.319	16.470	7.825		16.79 A
23											
	ATOM	1218	C	THR			79.069	17.195	5.980		17.35 A
	ATOM	1219	0	THR			79.246	18.062	5.130		16.83 A
	ATOM	1220	N	ASP			78.244	17.344	7.018		18.09 A
	ATOM	1221	CA	ASP	Α	223	77.466	18.567	7.268	1.00	19.60 A
30	MOTA	1222	CB	ASP	Α	223	78.403	19.778	7.311		22.73 A
	ATOM	1223	CG	ASP	Α	223	77.763	21.006	7.959	1.00	28.30 A
	ATOM	1224	OD1	ASP	Α	223	76.565	20.931	8.335		28.17 A
	ATOM	1225		ASP			78.480	22.042	8.081		30.99 A
	ATOM	1226	C	ASP			76.382	18.799	6.210		19.52 A
35	ATOM	1227	0	ASP			76.528	19.655	5.340		19.39 A
33											
	ATOM	1228	N	PHE			75.283	18.058	6.303		18.74 A
	ATOM	1229	CA	PHE			74.213	18.168	5.321		18.81 A
	MOTA	1230	СВ	PHE	Α	224	73.825	16.773	4.853	1.00	17.07 A
	ATOM	1231	CG	PHE	Α	224	74.857	16.150	3.971	1.00	17.01 A
40	ATOM	1232	CD1	PHE	Α	224	74.751	16.250	2.578	1.00	16.10 A
	ATOM	1233	CD2	PHE	Α	224	75.982	15.543	4.521	1.00	14.00 A
	ATOM	1234		PHE			75.761	15.752	1.747		15.92 A
	ATOM	1235		PHE			77.001	15.042	3.699		15.63 A
4.7	MOTA	1236	CZ			224	76.889	15.147			15.79 A
45	ATOM	1237	С	PHE			72.997	18.932	5.775		19.88 A
	ATOM	1238	0	PHE	Α	224	71.961	18.922	5.115	1.00	19.36 A
	MOTA	1239	N	GLY	Α	225	73.135	19.599	6.911	1.00	21.38 A
	MOTA	1240	CA	GLY	Α	225	72.046	20.388	7.439	1.00	21.39 A
	ATOM	1241	С	GLY	Α	225	71.672	21.545	6.523	1.00	23.43 A
50	ATOM	1242	0	GLY			70.802	22.323	6.869		26.22 A
20	ATOM	1243	N			226	72.311	21.692	5.370		22.15 A
	ATOM	1244	CA			226	71.930	22.784	4.492		23.85 A
	ATOM	1245	СВ	THR			72.986	23.946	4.465		24.65 A
	ATOM	1246		THR			74.197	23.511	3.830		24.83 A
55	ATOM	1247	CG2	THR	А	226	73.285	24.420	5.866	1.00	23.67 A
	MOTA	1248	C	THR	Α	226	71.721	22.289	3.073	1.00	24.12 A
	ATOM	1249	0	THR	Α	226	71.646	23.079	2.129	1.00	22.82 A
	ATOM	1250	N			227	71.620		2.935		23.84 A
	ATOM	1251		ALA			71.437	20.357	1.637		26.21 A
		1201	O2 1	4 144 1	- 1		. 1. 10 /	_0.507	1.007	00	A

	7) III () M	1252	CD	ALA .	70 0	227	71.774	18.889	1.734	1 00	24.04 A
	ATOM		СВ								
	ATOM	1253	C	ALA .			70.026	20.535	1.064		28.20 A
	MOTA	1254	0	ALA .			69.069	20.767	1.801		29.29 A
	MOTA	1255	N	ALA .			69.912	20.449	-0.258		28.91 A
5	ATOM	1256	CA	ALA .			68.623	20.554	-0.928		31.02 A
	MOTA	1257	СВ	ALA .	A 2	228	68.577	21.795	-1.856		30.45 A
	MOTA	1258	С	ALA .	A 2	228	68.501	19.276	-1.745	1.00	32.01 A
	ATOM	1259	0	ALA .	A 2	228	69.474	18.846	-2.363	1.00	32.87 A
	ATOM	1260	N	VAL .	A 2	229	67.328	18.650	-1.732	1.00	32.95 A
10	MOTA	1261	CA	VAL .	A 2	229	67.126	17.424	-2.503	1.00	34.26 A
	ATOM	1262	СВ	VAL .	A 2	229	66.468	16.347	-1.657	1.00	33.02 A
	ATOM	1263	CG1	VAL .	A 2	229	66.194	15.114	-2.498	1.00	33.80 A
	ATOM	1264	CG2	VAL .	A 2	229	67.356	16.011	-0.496	1.00	31.38 A
	ATOM	1265	С	VAL .			66.213	17.757	-3.665	1.00	36.36 A
15	ATOM	1266	0	VAL .			65.065	18.133	-3.455		38.02 A
	ATOM	1267	N	LEU .			66.715	17.628	-4.889		37.75 A
	ATOM	1268	CA	LEU .			65.917	17.965	-6.066		39.87 A
	ATOM	1269	CB	LEU .			66.741	17.775	-7.335		41.23 A
	ATOM	1270	CG	LEU .			68.039	18.585	-7.359		44.16 A
20	ATOM	1271		LEU .			68.843	18.208	-8.599		43.48 A
20	ATOM	1272		LEU .			67.724	20.087	-7.313		42.99 A
	ATOM	1273	C	LEU .			64.646	17.137	-6.162		40.59 A
	ATOM	1274	0	LEU .			64.703	15.954	-6.486		41.31 A
		1274		ASN .			65.964	27.756	-2.248		83.97 A
25	ATOM		N								
25	ATOM	1276	CA	ASN .			66.331 65.294	29.165	-2.370		84.48 A 85.56 A
	MOTA	1277	CB	ASN .				29.907	-3.225		
	ATOM	1278	CG	ASN .			63.949	30.053	-2.524		86.59 A
	ATOM	1279		ASN .			63.850	30.682	-1.465		87.31 A
20	ATOM	1280		ASN .			62.904	29.473	-3.115		86.14 A
30	ATOM	1281	C	ASN .			66.433	29.828	-0.994		83.85 A
	ATOM	1282	0	ASN .			66.898	30.963	-0.862		84.11 A
	ATOM	1283	N	ALA .			65.997	29.096	0.023		83.19 A
	MOTA	1284	CA	ALA .			65.996	29.564	1.405		81.85 A
	ATOM	1285	С	ALA .			67.330	29.365	2.127		79.97 A
35	MOTA	1286	0	ALA .			67.349	28.777	3.214		79.75 A
	ATOM	1287	СВ	ALA .			64.894	28.825	2.183	1.00	85.17 A
	ATOM	1288	N	PHE .			68.433	29.850	1.551		77.03 A
	ATOM	1289	CA	PHE .			69.737	29.680	2.197		74.85 A
	ATOM	1290	СВ	PHE .			69.973	28.183	2.438		73.81 A
40	ATOM	1291	CG	PHE .			71.311	27.861	3.015		72.36 A
	ATOM	1292		PHE .			71.595	28.116	4.353		72.39 A
	ATOM	1293	CD2				72.297	27.312	2.210		72.03 A
	ATOM	1294		PHE .			72.855	27.823	4.879		72.87 A
	MOTA	1295	CE2	PHE .			73.553	27.016	2.714		72.25 A
45	ATOM	1296	CZ	PHE .	A 2	242	73.837	27.270	4.054		72.96 A
	MOTA	1297	С	PHE .	A 2	242	70.951	30.283	1.462	1.00	73.13 A
	ATOM	1298	0	PHE .	A 2	242	70.958	30.425	0.233	1.00	74.08 A
	MOTA	1299	N	VAL .	A 2	243	71.972	30.625	2.250	1.00	69.64 A
	ATOM	1300	CA	VAL .	A 2	243	73.233	31.204	1.777	1.00	65.87 A
50	ATOM	1301	СВ	VAL .	A 2	243	73.207	32.765	1.834	1.00	66.73 A
	ATOM	1302	CG1	VAL .	A 2	243	74.498	33.344	1.271	1.00	65.65 A
	MOTA	1303	CG2	VAL .	A 2	243	72.008	33.299	1.084	1.00	66.83 A
	ATOM	1304	С	VAL .			74.349	30.708	2.703		62.21 A
	ATOM	1305	0	VAL .			74.471	31.189	3.839		61.91 A
55	ATOM	1306	N	GLY .			75.149	29.760	2.204		57.62 A
	ATOM	1307	CA	GLY .			76.247	29.177	2.967		51.60 A
	ATOM	1308	С	GLY .			77.341	30.132	3.387		46.47 A
	ATOM	1309	0	GLY .			77.063	31.261	3.757		48.62 A
	ATOM	1310	N	THR .			78.588	29.686	3.325		42.06 A
									5.525		

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	MOTA	1311	CA	THR			79.709	30.526	3.726		36.35 A
	MOTA	1312	СВ	THR	Α	245	80.925	29.673	4.096	1.00	35.76 A
	ATOM	1313	OG1	THR	Α	245	80.539	28.740	5.105	1.00	31.66 A
	ATOM	1314	CG2	THR	Α	245	82.043	30.534	4.651	1.00	33.72 A
5	ATOM	1315	С	THR			80.064	31.524	2.637		34.43 A
5		1316		THR			80.309				
	ATOM		0					31.166	1.485		33.95 A
	ATOM	1317	N	ALA			80.087	32.787	3.034		32.72 A
	ATOM	1318	CA	ALA	Α	246	80.338	33.900	2.142	1.00	30.18 A
	ATOM	1319	СВ	ALA	Α	246	80.684	35.127	2.952	1.00	30.18 A
10	ATOM	1320	С	ALA	Α	246	81.374	33.678	1.062	1.00	29.56 A
	ATOM	1321	0	ALA	A	246	81.099	33.895	-0.113	1.00	30.00 A
	ATOM	1322	N	GLN			82.564	33.242	1.445		28.03 A
	ATOM	1323	CA	GLN			83.623	33.030	0.468		26.97 A
	ATOM	1324	СВ	GLN			84.929	32.706	1.182		28.32 A
15	ATOM	1325	CG	GLN	Α	247	85.208	33.659	2.319	1.00	33.33 A
	MOTA	1326	CD	GLN	Α	247	86.600	33.522	2.863	1.00	36.16 A
	ATOM	1327	OE1	GLN	Α	247	87.556	34.107	2.335	1.00	36.68 A
	ATOM	1328	NE2	GLN	Α	247	86.738	32.731	3.922	1.00	39.27 A
	ATOM	1329	С	GLN			83.355	31.968	-0.583		25.04 A
20	ATOM	1330	0	GLN			83.962	31.997	-1.653		25.92 A
20	ATOM	1331		TYR			82.443	31.045	-0.304		22.51 A
			N								
	ATOM	1332	CA	TYR			82.161	29.970	-1.260		21.98 A
	ATOM	1333	СВ	TYR			82.273	28.613	-0.541		17.74 A
	ATOM	1334	CG	TYR	Α	248	83.626	28.444	0.117		14.83 A
25	MOTA	1335	CD1	TYR	Α	248	84.736	28.063	-0.630	1.00	14.53 A
	ATOM	1336	CE1	TYR	Α	248	86.017	28.034	-0.067	1.00	15.65 A
	ATOM	1337	CD2	TYR	Α	248	83.820	28.784	1.460	1.00	13.57 A
	ATOM	1338	CE2	TYR			85.086	28.757	2.039		13.28 A
	ATOM	1339	CZ	TYR			86.192	28.386	1.271		16.78 A
20											15.10 A
30	ATOM	1340	OH	TYR			87.471	28.411	1.816		
	MOTA	1341	С	TYR			80.827	30.091	-2.005		22.23 A
	ATOM	1342	0	TYR			80.523	29.268	-2.866		22.78 A
	ATOM	1343	N	VAL	Α	249	80.054	31.126	-1.680	1.00	21.81 A
	MOTA	1344	CA	VAL	Α	249	78.760	31.395	-2.308	1.00	22.22 A
35	ATOM	1345	СВ	VAL	Α	249	78.077	32.634	-1.640	1.00	22.82 A
	ATOM	1346	CG1	VAL	Α	249	76.904	33.139	-2.496	1.00	22.57 A
	ATOM	1347		VAL			77.606	32.270	-0.243		22.62 A
	ATOM	1348	C	VAL			78.878	31.666	-3.818		21.92 A
		1349		VAL			79.733	32.428	-4.255		20.01 A
40	ATOM		0								
40	ATOM	1350	N	SER			78.012	31.045	-4.609		22.88 A
	ATOM	1351	CA	SER			78.030	31.259	-6.049		24.81 A
	ATOM	1352	СВ	SER			77.357	30.105	-6.792	1.00	25.82 A
	MOTA	1353	OG	SER			75.999	29.984	-6.419	1.00	27.07 A
	ATOM	1354	С	SER	Α	250	77.288	32.546	-6.357	1.00	26.22 A
45	ATOM	1355	0	SER	Α	250	76.438	33.004	-5.582	1.00	25.88 A
	ATOM	1356	N	PRO			77.592	33.148	-7.506		26.70 A
	ATOM	1357	CD	PRO			78.632	32.813	-8.495		27.24 A
	ATOM	1358	CA	PRO			76.908	34.393	-7.847		27.21 A
50	ATOM	1359	CB	PRO			77.637	34.860	-9.113		25.51 A
50	ATOM	1360	CG	PRO			78.171	33.590	-9.701		27.43 A
	ATOM	1361	С	PRO	Α	251	75.399	34.288	-8.026	1.00	28.00 A
	MOTA	1362	0	PRO	Α	251	74.684	35.218	-7.678	1.00	28.30 A
	ATOM	1363	N	GLU	Α	252	74.908	33.166	-8.550	1.00	28.81 A
	ATOM	1364	CA	GLU	Α	252	73.469	33.012	-8.768	1.00	29.67 A
55	ATOM	1365	СВ	GLU			73.151	31.684	-9.463		29.72 A
	ATOM	1366	CG	GLU			73.698	30.453	-8.740		31.04 A
	ATOM	1367	CD	GLU			75.106	30.433	-9.191		30.61 A
		1368					75.880	30.073	-9.191 -9.597		30.55 A
	ATOM			GLU							
	ATOM	1369	OEZ	GLU	А	Z 3 Z	75.434	28.872	-9.130	1.00	30.80 A

	ATOM	1370	С	GLU A	. 252	72.709	33.083	-7.462	1.00 30.83 A
	ATOM	1371	0	GLU A	252	71.563	33.530	-7.423	1.00 31.87 A
	ATOM	1372	N	LEU A	253	73.351	32.639	-6.388	1.00 32.71 A
	ATOM	1373	CA	LEU A	253	72.734	32.655	-5.073	1.00 33.94 A
5	ATOM	1374	СВ	LEU A		73.612	31.901	-4.081	1.00 37.40 A
J									
	ATOM	1375	CG	LEU A		72.967	31.086	-2.950	1.00 41.64 A
	ATOM	1376		LEU A		72.067	31.925	-2.048	1.00 43.86 A
	ATOM	1377	CD2			72.144	30.017	-3.597	1.00 45.52 A
	ATOM	1378	С	LEU A	. 253	72.545	34.095	-4.603	1.00 35.67 A
10	ATOM	1379	0	LEU A	253	71.589	34.392	-3.897	1.00 37.48 A
	ATOM	1380	N	LEU A	254	73.451	34.989	-4.995	1.00 36.38 A
	ATOM	1381	CA	LEU A	254	73.372	36.397	-4.600	1.00 36.66 A
	ATOM	1382	СВ	LEU A	2.54	74.764	37.032	-4.572	1.00 33.81 A
	ATOM	1383	CG	LEU A		75.824	36.402	-3.674	1.00 33.40 A
15	ATOM	1384	CD1			77.183	37.022	-3.982	1.00 30.48 A
13									
	ATOM	1385	CD2	LEU A		75.440	36.574	-2.208	1.00 31.43 A
	ATOM	1386	С	LEU A		72.485	37.240	-5.511	1.00 38.89 A
	ATOM	1387	0	LEU A		72.079	38.328	-5.133	1.00 38.85 A
	ATOM	1388	N	THR A	255	72.187	36.754	-6.709	1.00 42.60 A
20	ATOM	1389	CA	THR A	255	71.358	37.528	-7.624	1.00 47.21 A
	ATOM	1390	СВ	THR A	255	72.102	37.847	-8.941	1.00 47.08 A
	ATOM	1391	OG1	THR A	255	72.008	36.718	-9.814	1.00 48.56 A
	ATOM	1392	CG2	THR A	255	73.581	38.157	-8.686	1.00 45.65 A
	ATOM	1393	C	THR A		70.044	36.848	-8.009	1.00 51.00 A
25	ATOM	1394	0	THR A		69.348	37.323	-8.903	1.00 51.80 A
23		1395	N	GLU A		69.696	35.745	-7.353	1.00 51.00 A
	ATOM								
	ATOM	1396	CA	GLU A		68.450	35.044	-7.683	1.00 58.97 A
	ATOM	1397	СВ	GLU A		68.679	34.057	-8.832	1.00 59.81 A
	MOTA	1398	CG	GLU A		68.922		-10.181	1.00 63.59 A
30	ATOM	1399	CD	GLU A		69.343	33.707	-11.240	1.00 65.64 A
	ATOM	1400	OE1	GLU A	. 256	68.727	32.617	-11.310	1.00 67.44 A
	ATOM	1401	OE2	GLU A	256	70.285	34.015	-12.007	1.00 66.61 A
	ATOM	1402	С	GLU A	256	67.859	34.279	-6.512	1.00 60.83 A
	ATOM	1403	0	GLU A		66.701	33.861	-6.563	1.00 61.27 A
35	ATOM	1404	N	ALA A		68.657	34.100	-5.463	1.00 62.31 A
	ATOM	1405	CA	ALA A		68.234	33.348	-4.285	1.00 63.29 A
	ATOM	1406	CB	ALA A		66.867	33.847	-3.784	1.00 62.76 A
									1.00 63.64 A
	ATOM	1407	C	ALA A		68.157	31.860	-4.651	
40	ATOM	1408	0	ALA A		67.790	31.028	-3.825	1.00 64.96 A
40	ATOM	1409	N	SER A		68.523	31.532	-5.888	1.00 62.79 A
	MOTA	1410	CA	SER A		68.485	30.150	-6.378	1.00 62.30 A
	MOTA	1411	СВ	SER A		68.049	30.144		1.00 63.00 A
	ATOM	1412	OG	SER A	. 258	68.762	31.129		1.00 63.40 A
	ATOM	1413	С	SER A	258	69.816	29.402	-6.237	1.00 61.09 A
45	ATOM	1414	0	SER A	258	70.862	30.009	-6.009	1.00 62.12 A
	ATOM	1415	N	ALA A	259	69.774	28.083	-6.389	1.00 58.47 A
	ATOM	1416	CA	ALA A		70.979	27.270	-6.278	1.00 55.79 A
	ATOM	1417	СВ	ALA A		71.403	27.164	-4.837	1.00 56.24 A
	ATOM	1418	C	ALA A		70.738	25.886	-6.842	1.00 53.38 A
50	ATOM	1419	0	ALA A		69.641	25.347	-6.736	1.00 54.10 A
50		1420	N	CYS A		71.768	25.347	-7.433	1.00 34.10 A
	ATOM								
	ATOM	1421	CA	CYS A		71.623	23.988	-8.015	1.00 45.68 A
	ATOM	1422	СВ	CYS A		71.067	24.106	-9.438	1.00 48.50 A
	MOTA	1423	SG	CYS A		69.936	22.732	-9.899	1.00 57.53 A
55	MOTA	1424	С	CYS A	260	72.980	23.318	-8.022	1.00 41.30 A
	MOTA	1425	0	CYS A	260	73.892	23.762	-7.335	1.00 39.24 A
	MOTA	1426	N	LYS A	261	73.118	22.258	-8.805	1.00 36.63 A
	MOTA	1427	CA	LYS A		74.369	21.535	-8.866	1.00 33.81 A
	ATOM	1428	СВ	LYS A		74.261	20.416	-9.897	1.00 34.27 A
				~ 1				2.00,	0 11

	ATOM	1429	CG	LYS	Α	261	73.250	19.362	-9.488	1.00	34.04 A
	ATOM	1430	CD	LYS	Α	261	72.995	18.353	-10.577	1.00	33.10 A
	ATOM	1431	CE	LYS			71.983		-10.105		32.48 A
_	MOTA	1432	NZ	LYS			71.660		-11.176		33.10 A
5	ATOM	1433	С	LYS	Α	261	75.565	22.419	-9.153	1.00	31.80 A
	ATOM	1434	0	LYS	Α	261	76.636	22.214	-8.589	1.00	31.89 A
	ATOM	1435	N	SER	Α	262	75.389	23.405	-10.025	1.00	29.92 A
	ATOM	1436	CA	SER			76.477		-10.354		28.19 A
	MOTA	1437	СВ	SER			76.034		-11.417		29.90 A
10	ATOM	1438	OG	SER	Α	262	76.184	24.732	-12.695	1.00	34.45 A
	ATOM	1439	С	SER	Α	262	77.047	25.069	-9.155	1.00	25.77 A
	ATOM	1440	0	SER	Α	262	78.225	25.405	-9.146	1.00	26.59 A
	ATOM	1441	N	SER			76.216	25.347	-8.159		23.42 A
	MOTA	1442	CA	SER			76.663	26.040	-6.953		23.04 A
15	ATOM	1443	СВ	SER	Α	263	75.502	26.209	-5.979	1.00	24.64 A
	ATOM	1444	OG	SER	Α	263	74.463	26.963	-6.572	1.00	31.12 A
	ATOM	1445	С	SER	Α	263	77.777	25.233	-6.283	1.00	21.37 A
	MOTA	1446	0	SER			78.745	25.803	-5.788		20.74 A
• •	ATOM	1447	N	ASP			77.640	23.909	-6.268		19.11 A
20	ATOM	1448	CA	ASP	Α	264	78.674	23.062	-5.682	1.00	19.35 A
	ATOM	1449	CB	ASP	Α	264	78.206	21.609	-5.579	1.00	18.45 A
	MOTA	1450	CG	ASP	Α	264	77.164	21.406	-4.500	1.00	19.39 A
	MOTA	1451		ASP			76.998	22.304	-3.649		20.34 A
		1452					76.522				
	MOTA			ASP				20.338	-4.488		19.48 A
25	ATOM	1453	С	ASP			79.943	23.127	-6.542		19.34 A
	ATOM	1454	0	ASP	Α	264	81.052	23.147	-6.018	1.00	20.70 A
	ATOM	1455	N	LEU	Α	265	79.772	23.162	-7.864	1.00	17.68 A
	ATOM	1456	CA	LEU	Α	265	80.898	23.232	-8.774	1.00	17.42 A
	ATOM	1457	СВ	LEU			80.406		-10.208		19.36 A
20											
30	MOTA	1458	CG	LEU			79.683		-10.453		19.53 A
	ATOM	1459	CD1	LEU	Α	265	79.189	21.655	-11.879	1.00	17.18 A
	ATOM	1460	CD2	LEU	Α	265	80.625	20.550	-10.168	1.00	14.91 A
	ATOM	1461	С	LEU	Α	265	81.619	24.566	-8.600	1.00	19.06 A
	ATOM	1462	0	LEU			82.850	24.649	-8.697		18.60 A
25											
35	MOTA	1463	N	TRP			80.853	25.621	-8.350		18.60 A
	MOTA	1464	CA	TRP	Α	266	81.468	26.902	-8.107		18.62 A
	ATOM	1465	CB	TRP	Α	266	80.405	27.976	-7.876	1.00	19.75 A
	ATOM	1466	CG	TRP	Α	266	80.997	29.277	-7.382	1.00	21.53 A
	ATOM	1467	CD2	TRP	Α	266	81.357	30.420	-8.174	1.00	22.40 A
40	ATOM	1468	CE2	TRP			81.917	31.375	-7.296		22.70 A
T U											
	MOTA	1469	CE3	TRP			81.260	30.728	-9.541		21.62 A
	ATOM	1470	CD1				81.344	29.582	-6.094		20.15 A
	ATOM	1471	NE1	TRP	Α	266	81.896	30.835	-6.037	1.00	20.80 A
	ATOM	1472	CZ2	TRP	Α	266	82.382	32.624	-7.739	1.00	22.47 A
45	ATOM	1473	C7.3	TRP	Α	266	81.721	31.961	-9.981	1.00	22.48 A
15		1474		TRP					-9.080		23.40 A
	ATOM						82.276	32.898			
	MOTA	1475	С	TRP			82.338	26.734	-6.857		18.89 A
	ATOM	1476	0	TRP	Α	266	83.523	27.070	-6.875	1.00	20.01 A
	ATOM	1477	N	ALA	Α	267	81.755	26.204	-5.780	1.00	16.09 A
50	MOTA	1478	CA	ALA	Α	267	82.502	25.994	-4.540	1.00	15.55 A
	ATOM	1479	СВ	ALA			81.630	25.313	-3.499		13.20 A
	MOTA	1480	С	ALA			83.738	25.145	-4.813		16.44 A
	MOTA	1481	0	ALA	Α	267	84.802	25.345	-4.218	1.00	17.65 A
	MOTA	1482	N	LEU	Α	268	83.597	24.181	-5.710	1.00	15.96 A
55	ATOM	1483	CA	LEU			84.732	23.336	-6.055		17.56 A
		1484	CB	LEU					-7.098		16.91 A
	ATOM						84.315	22.281			
	ATOM	1485	CG	LEU			85.477	21.535	-7.775		16.43 A
	ATOM	1486	CD1	LEU	Α	268	86.214	20.697	-6.766	1.00	15.17 A
	ATOM	1487	CD2	LEU	Α	268	84.947	20.643	-8.871	1.00	17.18 A

	ATOM	1488	С	LEU			85.892	24.193	-6.599		15.96 A	
	ATOM	1489	0	LEU			87.032	24.040	-6.178		14.54 A	
	MOTA	1490	N	$\operatorname{GL} Y$	Α	269	85.578	25.092	-7.530	1.00	17.15 A	7
	ATOM	1491	CA	GLY	Α	269	86.590	25.957	-8.116	1.00	18.32 A	4
5	ATOM	1492	С	GLY	Α	269	87.339	26.722	-7.042	1.00	19.39 A	7
	ATOM	1493	0	GLY			88.579	26.777	-7.042	1.00	19.66 A	4
	ATOM	1494	N	CYS			86.579	27.297	-6.111		17.50 A	
		1495	CA	CYS			87.154	28.043	-5.010		17.72 A	
	ATOM											
10	ATOM	1496	СВ	CYS			86.047	28.551	-4.088		18.96 A	
10	ATOM	1497	SG	CYS			84.981	29.801	-4.798		19.62 A	
	ATOM	1498	С	CYS			88.114	27.182	-4.201		18.63 A	
	ATOM	1499	0	CYS	Α	270	89.213	27.612	-3.850	1.00	18.78 A	7
	ATOM	1500	N	ILE	Α	271	87.679	25.962	-3.900	1.00	20.05 A	4
	ATOM	1501	CA	ILE			88.479	25.019	-3.130		20.08 A	
15	ATOM	1502	СВ	ILE			87.668	23.755	-2.812		20.09 A	
15	ATOM	1503	CG2	ILE			88.592	22.654	-2.302		18.31 A	
	ATOM	1504	CG1	ILE			86.558	24.104	-1.810		18.38 A	
	ATOM	1505	CD1	ILE			85.396	23.125	-1.783		14.68 A	
	ATOM	1506	С	ILE	Α	271	89.761	24.629	-3.858		20.41 A	
20	ATOM	1507	0	ILE	Α	271	90.826	24.548	-3.234	1.00	21.81 A	7
	ATOM	1508	N	ILE	Α	272	89.669	24.398	-5.166	1.00	18.41 A	Ā
	ATOM	1509	CA	ILE	Α	272	90.860	24.035	-5.934	1.00	19.20 A	Ā
	ATOM	1510	СВ	ILE			90.526	23.730	-7.412		20.04 A	
	ATOM	1511	CG2	ILE			91.808	23.488	-8.199		17.73 A	
25				ILE							19.47 P	
25	ATOM	1512	CG1				89.602	22.523	-7.513			
	ATOM	1513	CD1	ILE			89.001	22.386	-8.872		20.31 A	
	MOTA	1514	С	ILE			91.858	25.191	-5.932		19.57 A	
	ATOM	1515	0	ILE	Α	272	93.061	24.978	-5.884	1.00	20.97 A	7
	MOTA	1516	N	TYR	Α	273	91.338	26.413	-6.028	1.00	19.42 A	4
30	ATOM	1517	CA	TYR	Α	273	92.157	27.606	-6.041	1.00	18.41 A	Ā
	ATOM	1518	СВ	TYR			91.272	28.826	-6.294	1.00	18.70 A	Ā
	ATOM	1519	CG	TYR			91.998	30.147	-6.252		19.81 A	
	ATOM	1520	CD1	TYR			92.357	30.729	-5.035		21.25 A	
25	ATOM	1521	CE1	TYR			93.072	31.936	-4.990		22.12 P	
35	MOTA	1522	CD2	TYR			92.366	30.804	-7.433		20.45 A	
	ATOM	1523	CE2	TYR			93.081	32.005	-7.403		20.42 P	
	ATOM	1524	CZ	TYR	Α	273	93.432	32.563	-6.178	1.00	23.33 A	7
	MOTA	1525	OH	TYR	Α	273	94.159	33.731	-6.138	1.00	23.26 A	7
	ATOM	1526	С	TYR	Α	273	92.848	27.699	-4.687	1.00	19.40 A	7
40	ATOM	1527	0	TYR	Α	273	94.051	27.945	-4.598	1.00	19.44 A	4
	ATOM	1528	N	GLN	Α	274	92.079	27.471	-3.632	1.00	19.53 A	Ā
	ATOM	1529	CA	GLN			92.602	27.517	-2.278		21.26 P	
	ATOM	1530	СВ	GLN			91.450	27.399	-1.290		22.36 A	
	ATOM	1531	CG				91.838	27.629	0.142		21.87 A	
15				GLN								
45	MOTA	1532	CD	GLN			90.643	27.531	1.054		23.64 A	
	MOTA	1533		GLN			89.499	27.479	0.585		22.12 P	
	ATOM	1534	NE2	GLN	Α	274	90.890	27.517	2.369	1.00	24.45 A	7
	ATOM	1535	С	GLN	Α	274	93.656	26.435	-1.980	1.00	22.20 P	7
	ATOM	1536	0	GLN	Α	274	94.549	26.652	-1.160	1.00	22.03 P	7
50	ATOM	1537	N	LEU			93.558	25.275	-2.625	1.00	21.82 A	A
	MOTA	1538	CA	LEU			94.550	24.223	-2.385		21.95 A	
	ATOM	1539	СВ	LEU			94.104	22.886	-3.015		19.19 A	
	ATOM	1540	CG	LEU			92.934	22.153	-2.341		19.86 A	
	MOTA	1541		LEU			92.528	20.915	-3.134		19.79 A	
55	MOTA	1542	CD2	LEU			93.333	21.757	-0.938		16.56 A	
	MOTA	1543	С	LEU	Α	275	95.910	24.630	-2.962	1.00	21.62 P	1
	MOTA	1544	0	LEU	Α	275	96.950	24.414	-2.353	1.00	21.98 A	4
	ATOM	1545	N	VAL	Α	276	95.884	25.239	-4.137		20.54 A	
	ATOM	1546	CA	VAL			97.095	25.639	-4.828		21.48 A	
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	ATOM	1547	СВ	VAL	Α	276	96.810	25.795	-6.338		21.76 A	
	ATOM	1548	CG1	VAL	Α	276	98.035	26.269	-7.061	1.00	20.72 A	Ŧ
	ATOM	1549	CG2	VAL	Α	276	96.332	24.479	-6.908	1.00	21.98 A	1
	ATOM	1550	С	VAL	Α	276	97.696	26.946	-4.315	1.00	23.17 A	Į.
5	ATOM	1551	0	VAL			98.913	27.055	-4.141		24.82 A	
J	ATOM	1552	N	ALA			96.837	27.934	-4.085		22.20 A	
	ATOM	1553	CA	ALA			97.271	29.230	-3.628		19.31 A	
	ATOM	1554	СВ	ALA			96.339	30.293	-4.174		19.24 A	
	ATOM	1555	С	ALA			97.380	29.350	-2.113		20.10 A	
10	ATOM	1556	0	ALA	Α	277	98.096	30.222	-1.622	1.00	20.73 A	Ŧ
	ATOM	1557	N	GLY	Α	278	96.686	28.493	-1.368	1.00	19.16 A	ł
	ATOM	1558	CA	GLY	Α	278	96.748	28.579	0.084	1.00	18.62 A	Ł
	ATOM	1559	С	GLY	Α	278	95.634	29.425	0.677	1.00	21.09 A	Ā
	ATOM	1560	0	GLY			95.462	29.483	1.903		20.36 A	
15	ATOM	1561	N	LEU			94.865	30.084	-0.190		22.58 A	
13		1562		LEU			93.742	30.917	0.254		24.03 A	
	ATOM		CA									
	ATOM	1563	СВ	LEU			94.190	32.365	0.448		23.98 A	
	MOTA	1564	CG	LEU			95.322	32.744	1.396		25.93 A	
	ATOM	1565	CD1	LEU	Α	279	95.622	34.215	1.140		25.95 A	
20	ATOM	1566	CD2	LEU	Α	279	94.950	32.511	2.873	1.00	24.23 A	Ŧ
	ATOM	1567	С	LEU	Α	279	92.575	30.940	-0.735	1.00	23.96 A	Ł
	ATOM	1568	0	LEU	Α	279	92.759	30.776	-1.939	1.00	23.93 A	Ł
	ATOM	1569	N	PRO			91.353	31.151	-0.231	1.00	24.60 A	4
	ATOM	1570	CD	PRO			90.987	31.360	1.185		23.93 A	
25	ATOM	1571	CA	PRO			90.177	31.208	-1.109		24.56 A	
23		1572		PRO			89.024		-0.116			
	ATOM		CB					31.319			24.33 A	
	ATOM	1573	CG	PRO			89.656	32.027	1.076		24.23 A	
	MOTA	1574	С	PRO			90.324	32.453	-2.033		25.82 A	
	ATOM	1575	0	PRO	Α	280	90.892	33.458	-1.632		27.28 A	
30	ATOM	1576	N	PRO	Α	281	89.798	32.396	-3.268		25.40 A	
	ATOM	1577	CD	PRO	Α	281	88.807	31.385	-3.660	1.00	26.04 A	Ł
	ATOM	1578	CA	PRO	Α	281	89.862	33.470	-4.272	1.00	24.99 A	Ł
	ATOM	1579	СВ	PRO	Α	281	89.150	32.871	-5.489	1.00	24.76 A	Ā
	ATOM	1580	CG	PRO			88.882	31.442	-5.137		26.48 A	
35	ATOM	1581	C	PRO			89.254	34.836	-3.921		25.24 A	
33	ATOM	1582	0	PRO			89.803	35.886	-4.272		25.21 A	
	ATOM	1583	N	PHE			88.103	34.821	-3.264		24.47 A	
	ATOM	1584	CA	PHE			87.435	36.059	-2.918		24.29 A	
	MOTA	1585	СВ	PHE			85.964	35.961	-3.320		23.11 A	
40	ATOM	1586	CG	PHE			85.759	35.596	-4.774		21.99 A	
	MOTA	1587	CD1	PHE	Α	282	85.936	36.543	-5.775	1.00	20.97 A	1
	MOTA	1588	CD2	PHE	Α	282	85.448	34.285	-5.139	1.00	21.76 A	Ā
	ATOM	1589	CE1	PHE	Α	282	85.812	36.194	-7.124	1.00	20.59 A	Į.
	ATOM	1590	CE2	PHE	Α	282	85.325	33.923	-6.469	1.00	20.98 A	ł
45	ATOM	1591	CZ	PHE			85.509	34.885	-7.471		23.01 A	
	ATOM	1592	C	PHE			87.579	36.366	-1.435		25.85 A	
	ATOM	1593	0	PHE			86.963	35.707	-0.596		27.04 A	
	ATOM	1594	N	ARG			88.414	37.358	-1.124		27.56 A	
= 0	MOTA	1595	CA	ARG			88.676	37.784	0.260		27.41 A	
50	ATOM	1596	СВ	ARG			90.116	37.451	0.648		28.05 A	
	ATOM	1597	CG	ARG	Α	283	90.523	36.020	0.327		32.73 A	
	ATOM	1598	CD	ARG	Α	283	91.944	35.722	0.788	1.00	36.54 A	Ŧ
	ATOM	1599	NE	ARG	Α	283	92.942	36.490	0.043	1.00	39.92 A	ł
	ATOM	1600	CZ	ARG	Α	283	93.202	36.329	-1.253	1.00	42.59 A	Ŧ
55	ATOM	1601		ARG			92.544	35.421	-1.961		44.54 A	
	ATOM	1602		ARG			94.112	37.090	-1.853		43.94 A	
	ATOM	1603	C	ARG			88.445	39.291	0.394		27.01 A	
		1603	0	ARG			88.682	40.047			26.54 A	
	ATOM											
	ATOM	1605	N	ALA	А	∠04	87.977	39.724	1.568	1.00	26.05 A	7

	MOTA	1606	CA	ALA	Α	284	87.694	41.135	1.812	1.00	23.42 A	r
	ATOM	1607	СВ	ALA	Α	284	86.529	41.579	0.967	1.00	21.82 A	r
	ATOM	1608	С	ALA	Α	284	87.386	41.383	3.280	1.00	24.72 A	
	ATOM	1609	0	ALA			87.193	40.440	4.048		24.83 A	
5	ATOM	1610		GLY			87.330	42.663	3.659		25.04 A	
3			N									
	ATOM	1611	CA	GLY			87.055	43.039	5.035		23.67 A	
	ATOM	1612	С	GLY	Α	285	85.761	42.542	5.652	1.00	25.13 A	L
	MOTA	1613	0	GLY	Α	285	85.718	42.302	6.855	1.00	26.60 A	r
	ATOM	1614	N	ASN	Α	286	84.700	42.399	4.862	1.00	24.84 A	ı
10	ATOM	1615	CA	ASN			83.418	41.923	5.391	1.00	23.82 A	
	ATOM	1616	СВ	ASN			82.567	43.098	5.899		23.66 A	
	ATOM	1617	CG	ASN			82.362	44.190	4.843		24.14 A	
	ATOM	1618		ASN			81.835	43.947	3.747		22.27 A	
	MOTA	1619	ND2	ASN	Α	286	82.776	45.402	5.178	1.00	24.49 A	L
15	ATOM	1620	С	ASN	Α	286	82.672	41.185	4.296	1.00	24.75 A	7
	ATOM	1621	0	ASN	Α	286	83.124	41.160	3.153	1.00	25.32 A	
	ATOM	1622	N	GLU			81.522	40.610	4.630		26.04 A	
		1623									27.47 A	
	ATOM		CA	GLU			80.746	39.865	3.641			
	ATOM	1624	СВ	GLU			79.549	39.175	4.287		30.33 A	
20	MOTA	1625	CG	GLU	Α	287	79.935	38.202	5.364	1.00	36.51 A	7
	ATOM	1626	CD	GLU	Α	287	78.792	37.288	5.766	1.00	41.45 A	7
	ATOM	1627	OE1	GLU	Α	287	77.608	37.712	5.641	1.00	43.02 A	ī
	ATOM	1628	OE2	GLU	Α	287	79.092	36.155	6.222	1.00	41.33 A	
	ATOM	1629	C	GLU			80.250	40.679	2.467		25.95 A	
25	ATOM	1630	0	GLU			80.279	40.203	1.330		25.67 A	
23												
	ATOM	1631	N	TYR			79.772	41.893	2.730		25.20 A	
	ATOM	1632	CA	TYR			79.276	42.731	1.644		22.91 A	
	ATOM	1633	СВ	TYR			78.870	44.113	2.152		22.98 A	
	MOTA	1634	CG	TYR	Α	288	78.459	45.068	1.038	1.00	23.01 A	r
30	ATOM	1635	CD1	TYR	Α	288	77.166	45.031	0.478	1.00	24.16 A	r
	ATOM	1636	CE1	TYR	Α	288	76.814	45.869	-0.589	1.00	22.73 A	7
	ATOM	1637	CD2	TYR			79.376	45.965	0.508		21.34 A	
	ATOM	1638	CE2	TYR			79.043	46.796	-0.551		23.71 A	
	ATOM	1639	CZ	TYR			77.771	46.748	-1.099		25.48 A	
25												
35	ATOM	1640	OH	TYR			77.490	47.571	-2.172		26.98 A	
	ATOM	1641	С	TYR	Α	288	80.352	42.882	0.578		22.37 A	
	ATOM	1642	0	TYR	Α	288	80.068	42.735	-0.603	1.00	22.65 A	7
	ATOM	1643	N	LEU	Α	289	81.590	43.155	0.993	1.00	22.04 A	r
	ATOM	1644	CA	LEU	Α	289	82.691	43.326	0.037	1.00	23.92 A	٠
40	ATOM	1645	СВ	LEU			83.927	43.907	0.748		21.71 A	
10	ATOM	1646	CG	LEU			83.661	45.326	1.298		23.89 A	
											17.24 A	
	ATOM	1647		LEU			84.716	45.787	2.326			
	ATOM	1648		LEU					0.118		19.08 A	
	ATOM	1649	С			289	83.050	42.025			24.50 A	
45	MOTA	1650	0	LEU	Α	289	83.446	42.042	-1.852	1.00	24.85 A	L
	ATOM	1651	N	ILE	Α	290	82.906	40.904	-0.002	1.00	24.71 A	r
	ATOM	1652	CA	ILE	Α	290	83.182	39.601	-0.570	1.00	25.86 A	7
	ATOM	1653	СВ	ILE	Α	290	83.131	38.521	0.528		26.67 A	
	ATOM	1654		ILE			83.229	37.154	-0.087		27.57 A	
50												
50	ATOM	1655		ILE			84.282	38.736	1.511		28.90 A	
	ATOM	1656		ILE			84.173		2.798		28.83 A	
	ATOM	1657	С	ILE	А	290	82.127	39.303	-1.637	1.00	26.89 A	r
	MOTA	1658	0	ILE	Α	290	82.446	38.879	-2.757	1.00	26.18 A	L
	ATOM	1659	N	PHE	Α	291	80.864	39.531	-1.294	1.00	27.48 A	L
55	ATOM	1660	CA	PHE	Α	291	79.789	39.287	-2.249		28.46 A	
	ATOM	1661	СВ			291	78.434	39.587	-1.620		27.24 A	
	ATOM	1662	CG			291	78.079	38.664	-0.496		27.02 A	
	ATOM	1663		PHE			78.716	37.431			26.90 A	
							77.074		0.399		25.83 A	
	ATOM	1664	CDZ	PHE	А	∠ 9 ⊥	//.0/4	38.996	0.399	1.00	2J.03 A	L

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	ATOM	1665	CEI	PHE			78.353	36.545	0.637		27.02 A
	MOTA	1666	CE2	PHE	Α	291	76.700	38.109	1.412	1.00	28.02 A
	MOTA	1667	CZ	PHE	Α	291	77.338	36.882	1.532	1.00	26.74 A
	ATOM	1668	С	PHE	Α	291	79.971	40.159	-3.467	1.00	29.11 A
5	ATOM	1669	0	PHE			79.595	39.787	-4.584		30.18 A
5											
	ATOM	1670	N	GLN			80.559	41.324	-3.240		28.88 A
	ATOM	1671	CA	GLN	Α	292	80.783	42.280	-4.304		30.00 A
	ATOM	1672	СВ	GLN	Α	292	81.215	43.604	-3.679	1.00	32.57 A
	ATOM	1673	CG	GLN	Α	292	81.191	44.799	-4.599	1.00	35.12 A
10	ATOM	1674	CD	GLN	Α	292	81.208	46.113	-3.817		38.65 A
	ATOM	1675		GLN			82.159	46.409	-3.078		39.67 A
											38.94 A
	ATOM	1676		GLN			80.150	46.903	-3.972		
	ATOM	1677	С	GLN			81.822	41.755	-5.296		28.96 A
	MOTA	1678	0	GLN	Α	292	81.633	41.844	-6.510	1.00	28.45 A
15	MOTA	1679	N	LYS	Α	293	82.910	41.193	-4.787	1.00	26.32 A
	ATOM	1680	CA	LYS	Α	293	83.930	40.661	-5.669	1.00	26.90 A
	ATOM	1681	СВ	LYS			85.174	40.319	-4.858		28.03 A
	ATOM	1682	CG	LYS			85.777	41.539	-4.177		28.52 A
	ATOM	1683	CD	LYS			87.065	41.208	-3.482		29.14 A
20	ATOM	1684	CE	LYS	Α	293	87.912	42.449	-3.269	1.00	30.09 A
	ATOM	1685	NZ	LYS	Α	293	89.165	42.157	-2.490	1.00	30.06 A
	ATOM	1686	С	LYS	Α	293	83.414	39.432	-6.434	1.00	26.13 A
	ATOM	1687	0	LYS			83.721	39.231	-7.617		26.02 A
	ATOM	1688	N	ILE			82.617	38.621	-5.755		24.49 A
25											
25	ATOM	1689	CA	ILE			82.047	37.429	-6.362		24.40 A
	ATOM	1690	СВ	ILE	Α	294	81.168	36.680	-5.340		23.24 A
	MOTA	1691	CG2	ILE	Α	294	80.154	35.763	-6.046	1.00	21.00 A
	ATOM	1692	CG1	ILE	Α	294	82.072	35.929	-4.365	1.00	19.23 A
	ATOM	1693	CD1	ILE	Α	294	81.388	35.559	-3.067	1.00	17.91 A
30	ATOM	1694	С	ILE			81.224	37.744	-7.608		26.38 A
20	ATOM	1695	0	ILE			81.428	37.139	-8.661		25.96 A
		1696					80.303	38.694	-7.505		28.38 A
	ATOM		N	ILE							
	ATOM	1697	CA	ILE			79.467	39.018	-8.659		31.11 A
	ATOM	1698	СВ	ILE			78.243	39.852	-8.248		31.46 A
35	MOTA	1699	CG2	ILE	Α	295	77.548	39.181	-7.068		32.78 A
	MOTA	1700	CG1	ILE	Α	295	78.669	41.268	-7.871	1.00	31.79 A
	ATOM	1701	CD1	ILE	Α	295	77.518	42.132	-7.438	1.00	33.46 A
	ATOM	1702	С	ILE			80.201	39.731	-9.798		31.35 A
	ATOM	1703	0	ILE			79.709		-10.930		32.03 A
40											
40	ATOM	1704	N	LYS			81.374	40.269	-9.511		30.68 A
	ATOM	1705	CA	LYS			82.129		-10.552		31.64 A
	MOTA	1706	СВ	LYS	Α	296	82.683	42.275	-10.041		32.01 A
	MOTA	1707	CG	LYS	Α	296	81.605	43.213	-9.520	1.00	34.12 A
	MOTA	1708	CD	LYS	Α	296	82.184	44.441	-8.841	1.00	37.38 A
45	ATOM	1709	CE	LYS	Α	296	82.299	45.609	-9.803	1.00	40.30 A
	ATOM	1710	NΖ	LYS			82.864	46.819	-9.119		42.94 A
				LYS					-10.966		31.87 A
	ATOM	1711	С				83.258				
	ATOM	1712	0	LYS			84.135		-11.745		32.98 A
	ATOM	1713	N	LEU	Α	297	83.227	38.780	-10.443	1.00	30.62 A
50	MOTA	1714	CA	LEU	Α	297	84.253	37.775	-10.735	1.00	29.78 A
	MOTA	1715	СВ	LEU	Α	297	84.100	37.253	-12.169	1.00	29.42 A
	ATOM	1716	CG	LEU	Α	297	84.802		-12.527		29.13 A
	ATOM	1717		LEU			84.142		-11.783		27.91 A
	ATOM	1718		LEU			84.725		-14.024		26.86 A
55	ATOM	1719	С	LEU			85.622		-10.565		29.62 A
	ATOM	1720	0	LEU			86.489		-11.419		28.99 A
	ATOM	1721	N	GLU	Α	298	85.807	39.091	-9.427	1.00	29.81 A
	ATOM	1722	CA	GLU	Α	298	87.027	39.826	-9.143	1.00	30.88 A
	ATOM	1723	СВ	GLU			86.622	41.166	-8.510		33.22 A

	ATOM	1724	CG	GLU	Α	298	87.754	42.136	-8.228	1.00	38.19 A
	ATOM	1725	CD			298	87.317	43.274	-7.303		41.34 A
	ATOM	1726		GLU			86.416	44.054	-7.684		43.93 A
	MOTA	1727	OE2	GLU	Α	298	87.867	43.382	-6.187	1.00	43.19 A
5	ATOM	1728	С	GLU	Ά	298	88.071	39.110	-8.269	1.00	29.28 A
5											
	ATOM	1729	0	GLU			88.066	39.230	-7.045		30.04 A
	ATOM	1730	N	TYR	Α	299	88.972	38.375	-8.906	1.00	26.46 A
	ATOM	1731	CA	TYR	Α	299	90.034	37.669	-8.194	1.00	26.46 A
	ATOM	1732	СВ			299	89.548	36.315	-7.640		24.23 A
1.0											
10	ATOM	1733	CG	TYR	А	299	89.403	35.252	-8.709	1.00	23.32 A
	ATOM	1734	CD1	TYR	Α	299	88.369	35.318	-9.653	1.00	23.42 A
	ATOM	1735		TYR			88.274		-10.686		23.13 A
	ATOM	1736		TYR			90.337	34.227			21.77 A
	ATOM	1737	CE2	TYR	Α	299	90.250	33.292	-9.864	1.00	21.81 A
15	ATOM	1738	CZ	TYR	Α	299	89.214	33.379	-10.784	1.00	22.35 A
	ATOM	1739	ОН			299	89.089		-11.780		21.61 A
	ATOM	1740	С	TYR	А	299	91.102	37.416	-9.245	1.00	28.31 A
	ATOM	1741	0	TYR	Α	299	90.864	37.622	-10.426	1.00	27.25 A
	ATOM	1742	N			300	92.277	36.959			30.57 A
20							93.282	36.687			
20	ATOM	1743	CA			300			-9.851		33.57 A
	ATOM	1744	СВ	ASP	Α	300	94.012	37.980	-10.193	1.00	38.77 A
	ATOM	1745	CG	ASP	Α	300	94.382	38.768	-8.968	1.00	43.17 A
	ATOM	1746		ASP			95.245	38.283	-8.197		46.59 A
	ATOM	1747		ASP			93.802	39.865	-8.773		45.78 A
25	ATOM	1748	С	ASP	Α	300	94.232	35.607	-9.364	1.00	33.20 A
	ATOM	1749	0	ASP	Α	300	94.311	35.354	-8.169	1.00	33.46 A
	ATOM	1750	N			301	94.937		-10.287		32.16 A
	ATOM	1751	CA			301	95.853	33.892			33.41 A
	MOTA	1752	CB	PHE	Α	301	95.922	32.813	-11.001	1.00	32.89 A
30	ATOM	1753	CG	PHE	Ά	301	94.590	32.240	-11.403	1.00	33.05 A
20											
	ATOM	1754		PHE			93.763		-12.297		31.61 A
	ATOM	1755	CD2	PHE	Α	301	94.171	31.006	-10.905	1.00	30.94 A
	ATOM	1756	CE1	PHE	Α	301	92.548	32.387	-12.687	1.00	31.29 A
	ATOM	1757		PHE			92.961		-11.287		31.42 A
25											
35	ATOM	1758	CZ			301	92.142		-12.184		32.69 A
	MOTA	1759	С	PHE	Α	301	97.287	34.359	-9.649	1.00	34.23 A
	ATOM	1760	0	PHE	Α	301	97.784	35.274	-10.303	1.00	33.66 A
	ATOM	1761	N	DRO	7\	302	97.962	33.750	-8.665		35.45 A
	ATOM	1762	CD			302	97.426	32.932	-7.564		35.55 A
40	ATOM	1763	CA	PRO	Α	302	99.347	34.145	-8.395	1.00	35.82 A
	ATOM	1764	СВ	PRO	Α	302	99.612	33.571	-7.009	1.00	35.09 A
	ATOM	1765	CG			302	98.682	32.401	-6.933		34.93 A
	ATOM	1766	С	PRO			100.214	33.506	-9.485		37.48 A
	ATOM	1767	0	PRO	Α	302	99.830	32.504	-10.083	1.00	37.30 A
45	ATOM	1768	N	ALA	Α	303	101.370	34.100	-9.744	1.00	39.16 A
	ATOM	1769	CA	ALA			102.293		-10.775		39.50 A
	ATOM	1770	СВ	ALA			103.612		-10.640		39.58 A
	MOTA	1771	С	ALA	Α	303	102.577	32.148	-10.832	1.00	41.05 A
	ATOM	1772	0	ALA	Α	303	102.642	31.569	-11.920	1.00	42.39 A
50	ATOM	1773	N	ALA			102.758	31.526	-9.671		40.38 A
50											
	MOTA	1774	CA	ALA	Α	304	103.099	30.105	-9.614	1.00	39.93 A
	MOTA	1775	CB	ALA	Α	304	103.627	29.772	-8.212	1.00	41.64 A
	ATOM	1776	С	ALA			102.025		-10.002		38.27 A
= =	ATOM	1777	0	ALA			102.343		-10.453		39.29 A
55	ATOM	1778	N	PHE	Α	305	100.764	29.453	-9.813	1.00	35.83 A
	ATOM	1779	CA	PHE	Α	305	99.614	28.587	-10.085	1.00	33.62 A
	ATOM	1780	СВ			305	98.376		-10.278		32.70 A
	ATOM	1781	CG			305	97.096		-9.796		31.41 A
	MOTA	1782	CD1	PHE	Α	305	96.422	27.915	-10.574	1.00	30.30 A

					_						
	MOTA	1783		PHE			96.556	29.225	-8.562		30.99 A
	ATOM	1784	CE1	PHE	Α	305	95.230	27.350	-10.136	1.00	29.76 A
	MOTA	1785	CE2	PHE	Α	305	95.352	28.663	-8.105	1.00	30.08 A
	ATOM	1786	CZ	PHE	Α	305	94.689	27.725	-8.897	1.00	30.22 A
5	ATOM	1787	С	PHE	Α	305	99.735	27.580	-11.241	1.00	32.03 A
	ATOM	1788	0	PHE			99.767		-12.405		32.54 A
	ATOM	1789	N	PHE			99.781		-10.914		31.58 A
	ATOM	1790	CA	PHE			99.886		-11.932		30.32 A
• •	ATOM	1791	СВ	PHE			99.518		-11.338		29.86 A
10	ATOM	1792	CG	PHE	Α	306	100.087	23.639	-9.971		30.29 A
	ATOM	1793	CD1	PHE	Α	306	101.447	23.783	-9.733	1.00	30.37 A
	ATOM	1794	CD2	PHE	Α	306	99.259	23.275	-8.919	1.00	30.23 A
	ATOM	1795	CE1	PHE	Α	306	101.975	23.570	-8.465	1.00	30.98 A
	ATOM	1796	CE2	PHE	Α	306	99.773	23.061	-7.648		30.91 A
15	ATOM	1797	CZ	PHE			101.136	23.210	-7.418		31.14 A
13		1798	C	PHE			98.949		-13.096		29.48 A
	ATOM										
	ATOM	1799	0	PHE			97.738		-12.920		30.39 A
	ATOM	1800	N	PRO			99.501		-14.309		28.76 A
	ATOM	1801	CD	PRO			100.934	25.575	-14.635		27.67 A
20	ATOM	1802	CA	PRO	Α	307	98.731	26.014	-15.520	1.00	27.24 A
	ATOM	1803	СВ	PRO	Α	307	99.757	25.848	-16.635	1.00	25.23 A
	ATOM	1804	CG	PRO	Α	307	101.010	26.262	-15.978	1.00	25.61 A
	ATOM	1805	С	PRO			97.457	25.221	-15.787		25.86 A
	ATOM	1806	0	PRO			96.419		-16.098		24.65 A
25	ATOM	1807	N	LYS			97.521		-15.682		25.13 A
23											
	ATOM	1808	CA	LYS			96.330		-15.952		24.53 A
	ATOM	1809	СВ	LYS			96.689		-16.136		24.86 A
	ATOM	1810	CG	LYS			97.361		-17.490	1.00	25.50 A
	ATOM	1811	CD	LYS	Α	308	97.987	20.047	-17.616	1.00	27.33 A
30	ATOM	1812	CE	LYS	Α	308	98.678	19.886	-18.961	1.00	29.39 A
	ATOM	1813	NZ	LYS	Α	308	99.232	18.505	-19.146	1.00	32.38 A
	ATOM	1814	С	LYS	Α	308	95.282	23,293	-14.890	1.00	24.82 A
	ATOM	1815	0	LYS			94.085		-15.193		24.89 A
	ATOM	1816	N	ALA			95.716		-13.647		24.73 A
35							94.758		-12.573		25.03 A
33	ATOM	1817	CA	ALA							
	ATOM	1818	СВ	ALA			95.445		-11.208		24.10 A
	MOTA	1819	С	ALA			94.140		-12.816		25.34 A
	ATOM	1820	0	ALA	Α	309	92.934	25.273	-12.679		26.34 A
	ATOM	1821	N	ARG	Α	310	94.958	26.067	-13.198	1.00	26.07 A
40	ATOM	1822	CA	ARG	Α	310	94.419	27.396	-13.453	1.00	28.32 A
	ATOM	1823	СВ	ARG	Α	310	95.513	28.359	-13.908	1.00	29.31 A
	ATOM	1824	CG	ARG			94.940	29.708	-14.288	1.00	31.58 A
	ATOM	1825	CD	ARG			95.917		-15.030		31.47 A
	ATOM	1826	NE	ARG			95.275		-15.473		34.52 A
45	ATOM	1827	CZ	ARG			95.771		-15.276		35.51 A
43											
	ATOM	1828		ARG			96.929		-14.633		33.99 A
	ATOM	1829		ARG			95.106		-15.720		32.10 A
	MOTA	1830	С	ARG	Α	310	93.331	27.348	-14.521		29.03 A
	ATOM	1831	0	ARG	Α	310	92.308	28.034	-14.418	1.00	29.32 A
50	ATOM	1832	N	ASP	Α	311	93.548	26.536	-15.551	1.00	29.06 A
	ATOM	1833	CA	ASP	Α	311	92.571	26.432	-16.620	1.00	29.87 A
	ATOM	1834	СВ	ASP			93.156		-17.776		31.71 A
	ATOM	1835	CG	ASP			92.207		-18.953		34.71 A
<i>5 5</i>	ATOM	1836		ASP			91.288		-18.912		36.90 A
55	ATOM	1837		ASP			92.378		-19.918		36.33 A
	MOTA	1838	С	ASP			91.264		-16.128		29.70 A
	ATOM	1839	0	ASP	А	311	90.169	26.238	-16.513		29.95 A
	ATOM	1840	N	LEU	Α	312	91.383	24.778	-15.282	1.00	26.64 A
	MOTA	1841	CA	LEU	Α	312	90.215	24.112	-14.715	1.00	24.92 A

	ATOM	1842	СВ	LEU A	212	90.645	22.911 -13.869	1.00 23.93 A
		1843						
	MOTA		CG	LEU A		89.504	22.112 -13.227	1.00 24.48 A
	ATOM	1844		LEU A		88.569	21.610 -14.296	1.00 25.07 A
_	ATOM	1845		LEU A		90.061	20.945 -12.460	1.00 25.13 A
5	MOTA	1846	С	LEU A		89.412	25.095 -13.841	1.00 23.85 A
	MOTA	1847	0	LEU A		88.182	25.136 -13.896	1.00 21.21 A
	MOTA	1848	N	VAL A		90.121	25.886 -13.042	1.00 23.12 A
	MOTA	1849	CA	VAL A	313	89.484	26.865 -12.171	1.00 23.55 A
	ATOM	1850	СВ	VAL A	313	90.536	27.583 -11.297	1.00 22.33 A
10	ATOM	1851	CG1	VAL A	313	89.898	28.752 -10.559	1.00 19.05 A
	ATOM	1852	CG2	VAL A	313	91.144	26.607 -10.305	1.00 19.89 A
	ATOM	1853	С	VAL A	313	88.701	27.915 -12.975	1.00 25.59 A
	ATOM	1854	0	VAL A	313	87.590	28.305 -12.605	1.00 26.57 A
	ATOM	1855	N	GLU A		89.278	28.378 -14.076	1.00 26.08 A
15	ATOM	1856	CA	GLU A		88.598	29.370 -14.895	1.00 26.79 A
10	ATOM	1857	СВ	GLU A		89.543	29.928 -15.948	1.00 27.50 A
	ATOM	1858	CG	GLU A		90.739	30.639 -15.381	1.00 32.29 A
	ATOM	1859	CD	GLU A		91.687	31.094 -16.463	1.00 35.85 A
	ATOM	1860		GLU A		91.967	30.280 -17.375	1.00 35.05 A
20		1861	OE 2	GLU A		92.157	32.257 -16.399	1.00 38.08 A
20	ATOM ATOM	1862		GLU A		87.370	28.787 -15.577	
			C					1.00 26.22 A
	ATOM	1863	0	GLU A		86.499	29.527 -16.038	1.00 27.23 A
	ATOM	1864	N	LYS A		87.300	27.464 -15.662	1.00 24.74 A
2.5	ATOM	1865	CA	LYS A		86.151	26.832 -16.294	1.00 23.60 A
25	ATOM	1866	СВ	LYS A		86.578	25.584 -17.073	1.00 23.69 A
	ATOM	1867	CG	LYS A		87.393	25.865 -18.344	1.00 22.41 A
	ATOM	1868	CD	LYS A		87.825	24.545 -18.968	1.00 25.68 A
	ATOM	1869	CE	LYS A		88.768	24.695 -20.155	1.00 24.86 A
	ATOM	1870	NZ	LYS A		88.082	25.219 -21.346	1.00 28.62 A
30	MOTA	1871	С	LYS A		85.119	26.471 -15.230	1.00 23.42 A
	ATOM	1872	0	LYS A	315	84.043	25.970 -15.541	1.00 25.37 A
	MOTA	1873	N	LEU A	316	85.454	26.730 -13.970	1.00 21.88 A
	MOTA	1874	CA	LEU A	316	84.549	26.461 -12.862	1.00 20.21 A
	MOTA	1875	СВ	LEU A	316	85.272	25.705 -11.767	1.00 19.57 A
35	ATOM	1876	CG	LEU A	316	85.409	24.221 -12.078	1.00 21.14 A
	MOTA	1877	CD1	LEU A	316	86.272	23.552 -11.009	1.00 19.21 A
	ATOM	1878	CD2	LEU A	316	84.000	23.600 -12.166	1.00 18.59 A
	ATOM	1879	С	LEU A	316	83.996	27.758 -12.290	1.00 21.31 A
	ATOM	1880	0	LEU A	316	82.811	27.848 -11.955	1.00 18.79 A
40	ATOM	1881	N	LEU A		84.865	28.762 -12.175	1.00 20.59 A
	ATOM	1882	CA	LEU A		84.446	30.038 -11.646	1.00 21.64 A
	ATOM	1883	СВ	LEU A		85.606	30.707 -10.900	1.00 21.42 A
	ATOM	1884	CG	LEU A		86.130	29.892 -9.711	1.00 21.80 A
	ATOM	1885		LEU A		87.299	30.599 -9.047	1.00 23.09 A
45	ATOM	1886		LEU A		85.031	29.688 -8.724	1.00 20.34 A
15	ATOM	1887	C	LEU A		83.940	30.890 -12.810	1.00 23.34 A
	ATOM	1888	0	LEU A		84.568	31.859 -13.242	1.00 23.34 A
	ATOM	1889	N	VAL A		82.786	30.485 -13.324	1.00 23.29 A 1.00 24.06 A
		1890	CA				31.161 -14.436	
50	ATOM			VAL A		82.135	30.150 -15.547	1.00 23.46 A
50	ATOM	1891	CB	VAL A		81.829		1.00 24.32 A
	MOTA	1892		VAL A		81.061	30.828 -16.670	1.00 22.57 A
	ATOM	1893		VAL A		83.136	29.524 -16.049	1.00 20.68 A
	MOTA	1894	С	VAL A		80.838	31.765 -13.918	1.00 24.59 A
	ATOM	1895	0	VAL A		80.050	31.086 -13.250	1.00 24.86 A
55	ATOM	1896	N	LEU A		80.603	33.036 -14.215	1.00 24.95 A
	ATOM	1897	CA	LEU A		79.383	33.688 -13.731	1.00 25.79 A
	MOTA	1898	СВ	LEU A		79.379	35.157 -14.154	1.00 25.38 A
	MOTA	1899	CG	LEU A	319	80.466	35.963 -13.417	1.00 27.04 A
	MOTA	1900	CD1	LEU A	319	80.452	37.421 -13.869	1.00 25.54 A

	7.50.7.5	1001	an.o	T 1777	_	210	00 041	25 070	11 007	1 00	00 07	70
	ATOM	1901		LEU			80.241		-11.907		23.27	
	ATOM	1902	С	LEU			78.077		-14.141		26.05	
	ATOM	1903	0	LEU			77.171		-13.319		27.69	
	MOTA	1904	N	ASP	Α	320	77.982	32.580	-15.400	1.00	25.08	Α
5	ATOM	1905	CA	ASP	Α	320	76.804	31.881	-15.892	1.00	24.00	Α
	ATOM	1906	СВ	ASP	Α	320	76.788	31.907	-17.420	1.00	24.02	Α
	ATOM	1907	CG	ASP	Α	320	75.597	31.175	-17.996	1.00	27.27	Α
	ATOM	1908		ASP			75.009		-17.271		29.66	
	ATOM	1909		ASP			75.253		-19.175		30.03	
10	ATOM	1910	C	ASP			76.846		-15.396		24.04	
10												
	ATOM	1911	0	ASP			77.661		-15.846		25.11	
	ATOM	1912	N	ALA			75.940		-14.489		23.73	
	ATOM	1913	CA	ALA			75.867		-13.887		23.58	
	MOTA	1914	СВ	ALA	Α	321	74.710	28.720	-12.916	1.00	23.62	Α
15	ATOM	1915	С	ALA	Α	321	75.765	27.599	-14.853	1.00	24.90	Α
	MOTA	1916	0	ALA	Α	321	76.221	26.497	-14.549	1.00	24.36	Α
	ATOM	1917	N	THR	Α	322	75.176	27.834	-16.019	1.00	25.50	Α
	ATOM	1918	CA	THR			75.008		-17.011		24.60	
	ATOM	1919	СВ	THR			73.816		-17.909		23.09	
20	ATOM	1920		THR			74.079		-18.646		23.74	
20		1921							-17.080			
	ATOM			THR			72.568				20.71	
	ATOM	1922	С	THR			76.238		-17.893		25.24	
	ATOM	1923	0	THR			76.221		-18.832		26.45	
	ATOM	1924	N	LYS	Α	323	77.300		-17.592		25.05	
25	MOTA	1925	CA	LYS	Α	323	78.526	27.239	-18.366	1.00	26.46	Α
	ATOM	1926	CB	LYS	Α	323	78.972	28.627	-18.823	1.00	28.68	Α
	ATOM	1927	CG	LYS	Α	323	78.050	29.304	-19.814	1.00	31.27	Α
	ATOM	1928	CD	LYS	Α	323	78.470	29.004	-21.240	1.00	34.38	Α
	ATOM	1929	CE	LYS			77.850		-22.243		35.12	
30	ATOM	1930	NZ	LYS			76.363		-22.251		36.71	
30	ATOM	1931	C	LYS			79.660		-17.556		26.39	
	ATOM	1932	0	LYS			80.795		-18.010		28.51	
	ATOM	1933	N	ARG			79.372		-16.360		24.50	
	ATOM	1934	CA	ARG			80.429		-15.543		23.37	
35	ATOM	1935	СВ	ARG			80.087		-14.049		23.41	
	MOTA	1936	CG	ARG	Α	324	80.233	27.034	-13.520	1.00	21.60	Α
	ATOM	1937	CD	ARG	Α	324	79.594	27.220	-12.173	1.00	21.55	Α
	ATOM	1938	NE	ARG	Α	324	79.245	28.624	-11.986	1.00	19.69	Α
	ATOM	1939	CZ	ARG	Α	324	78.273	29.054	-11.191	1.00	19.84	Α
40	ATOM	1940	NH1	ARG	Α	324	77.555		-10.496	1.00	16.83	Α
	ATOM	1941		ARG			77.990		-11.129		21.41	
	ATOM	1942	С	ARG			80.717		-15.897		22.63	
	ATOM	1943	0	ARG			79.798		-16.058		24.44	
45	ATOM	1944	N	LEU			82.000		-16.023		20.68	
45	ATOM	1945	CA	LEU			82.414		-16.352		20.98	
	ATOM	1946	СВ	LEU			83.952		-16.386		20.82	
	ATOM	1947	CG	LEU			84.596		-17.131		23.08	
	MOTA	1948	CD1	LEU	Α	325	84.149	21.194	-18.595	1.00	21.39	Α
	ATOM	1949	CD2	LEU	Α	325	86.132	21.173	-17.038	1.00	20.00	Α
50	ATOM	1950	С	LEU	Α	325	81.840	21.454	-15.290	1.00	20.43	Α
	ATOM	1951	0	LEU	Α	325	82.062		-14.097	1.00	18.45	Α
	ATOM	1952	N	GLY			81.076		-15.725		21.33	
	ATOM	1953	CA	GLY			80.501		-14.778		20.60	
55	ATOM	1954	C	GLY			78.984		-14.701		22.39	
55	ATOM	1955	0	GLY			78.383		-14.378		22.59	
	ATOM	1956	N	CYS			78.358		-15.009		23.36	
	ATOM	1957	CA	CYS			76.896		-14.963		25.18	
	ATOM	1958	СВ	CYS			76.453		-14.889		25.79	
	ATOM	1959	SG	CYS	Α	327	76.742	23.237	-16.364	1.00	31.42	Α

	ATOM	1960	С	CYS A	227	76.229	20.074 -16.148	1.00 24.99 A
						76.887	19.743 -17.129	
	ATOM	1961	0	CYS A				1.00 24.31 A
	ATOM	1962	N	ALA A		74.923	19.847 -16.040	1.00 26.34 A
_	MOTA	1963	CA	ALA A		74.157	19.172 -17.094	1.00 27.51 A
5	MOTA	1964	СВ	ALA A		72.703	18.949 -16.629	1.00 26.81 A
	ATOM	1965	С	ALA A		74.179	19.905 -18.443	1.00 28.11 A
	ATOM	1966	0	ALA A	328	74.243	19.274 -19.501	1.00 27.66 A
	MOTA	1967	N	GLU A	329	74.144	21.231 -18.418	1.00 28.05 A
	MOTA	1968	CA	GLU A	329	74.172	21.973 -19.668	1.00 29.54 A
10	ATOM	1969	СВ	GLU A	329	73.915	23.458 -19.428	1.00 32.18 A
	ATOM	1970	CG	GLU A	329	72.539	23.783 -18.863	1.00 37.89 A
	ATOM	1971	CD	GLU A	329	72.418	23.503 -17.374	1.00 41.37 A
	ATOM	1972		GLU A		73.464	23.308 -16.711	1.00 43.80 A
	ATOM	1973	OE2	GLU A		71.273	23.495 -16.863	1.00 43.66 A
15	ATOM	1974	C	GLU A		75.514	21.807 -20.377	1.00 49.00 A
13	ATOM	1975	0	GLU A		75.602	21.927 -21.605	1.00 29.00 A
	ATOM	1976	N	MET A		76.559	21.540 -19.598	1.00 27.54 A
	ATOM	1977	CA	MET A		77.894	21.359 -20.148	1.00 25.71 A
	MOTA	1978	СВ	MET A		78.945	21.963 -19.219	1.00 27.88 A
20	MOTA	1979	CG	MET A		78.964	23.489 -19.209	1.00 30.29 A
	MOTA	1980	SD	MET A		79.429	24.194 -20.819	1.00 34.04 A
	MOTA	1981	CE	MET A	330	81.187	23.670 -20.936	1.00 29.55 A
	MOTA	1982	С	MET A	330	78.156	19.884 -20.343	1.00 24.53 A
	ATOM	1983	0	MET A	330	79.290	19.473 -20.575	1.00 22.65 A
25	ATOM	1984	N	GLU A	331	77.089	19.095 -20.221	1.00 22.87 A
	ATOM	1985	CA	GLU A	331	77.139	17.654 -20.415	1.00 21.38 A
	ATOM	1986	СВ	GLU A	331	77.854	17.339 -21.735	1.00 22.71 A
	ATOM	1987	CG	GLU A		76.903	16.916 -22.837	1.00 23.01 A
	ATOM	1988	CD	GLU A		75.599	17.720 -22.875	1.00 24.76 A
30	ATOM	1989		GLU A		75.570	18.830 -23.441	1.00 26.12 A
30	ATOM	1990		GLU A		74.588	17.230 -22.337	1.00 20.12 A
	ATOM	1991	C	GLU A		77.671	16.765 -19.290	1.00 21.01 A
	ATOM	1992	0	GLU A		78.075	15.619 -19.517	1.00 19.50 A
	ATOM	1993	N	GLY A		77.675	17.284 -18.071	1.00 19.73 A
35	ATOM	1994	CA	GLY A		78.056	16.445 -16.954	1.00 17.80 A
	MOTA	1995	С	GLY A		79.494	16.243 -16.570	1.00 17.28 A
	ATOM	1996	0	GLY A	332	80.381	17.013 -16.934	1.00 16.11 A
	MOTA	1997	N	TYR A	333	79.701	15.151 -15.842	1.00 16.52 A
	ATOM	1998	CA	TYR A	333	80.997	14.791 -15.305	1.00 16.75 A
40	ATOM	1999	СВ	TYR A	333	80.787	13.854 -14.115	1.00 16.95 A
	MOTA	2000	CG	TYR A	333	80.369	14.624 -12.893	1.00 18.08 A
	ATOM	2001	CD1	TYR A	333	81.332	15.207 -12.059	1.00 18.77 A
	ATOM	2002		TYR A		80.971	16.035 -10.982	1.00 17.69 A
	ATOM	2003		TYR A		79.021	14.877 -12.620	1.00 17.08 A
45	ATOM	2004		TYR A		78.646	15.713 -11.538	1.00 19.05 A
15	ATOM	2005	CZ	TYR A		79.640	16.287 -10.728	1.00 18.04 A
		2006	OH	TYR A		79.322		1.00 18.69 A
	ATOM	2007					17.126 -9.682 14.240 -16.238	
	ATOM		C	TYR A		82.051		1.00 16.78 A
50	ATOM	2008	0	TYR A		83.248	14.393 -15.977	1.00 16.04 A
50	ATOM	2009	N	GLY A		81.633	13.598 -17.321	1.00 16.63 A
	MOTA	2010	CA	GLY A		82.624	13.082 -18.244	1.00 17.02 A
	MOTA	2011	С	GLY A		83.576	14.194 -18.683	1.00 17.47 A
	MOTA	2012	0	GLY A	334	84.802	14.063 -18.562	1.00 17.18 A
	MOTA	2013	N	PRO A		83.039	15.315 -19.195	1.00 17.04 A
55	MOTA	2014	CD	PRO A	335	81.650	15.611 -19.590	1.00 16.18 A
	ATOM	2015	CA	PRO A		83.940	16.382 -19.621	1.00 17.35 A
	ATOM	2016	СВ	PRO A		82.991	17.441 -20.178	1.00 17.48 A
	ATOM	2017	CG	PRO A		81.857	16.605 -20.713	1.00 18.64 A
	ATOM	2018	C	PRO A		84.786	16.883 -18.480	1.00 18.48 A
	111 011	2010	_	II.O A	555	31.700	10.000 10.100	1.00 10.10 A

		ATOM	2019	0	PRO A	A	335	85.963	17.131	-18.661	1.00	20.84 A
		ATOM	2020	N	LEU Z			84.204		-17.299		19.46 A
		ATOM	2021	CA	LEU Z			84.986		-16.153		19.38 A
		ATOM	2022	СВ	LEU Z	A	336	84.071	17.692	-14.937		18.98 A
	5	ATOM	2023	CG	LEU Z	A	336	84.765		-13.604	1.00	18.01 A
		ATOM	2024	CD1	LEU Z			85.534	19.289	-13.690		16.66 A
		ATOM	2025		LEU Z			83.724	18.055	-12.491		18.81 A
		ATOM	2026	С	LEU Z	A	336	86.132	16.528	-15.815	1.00	19.32 A
		ATOM	2027	0	LEU Z	A	336	87.293	16.932	-15.683	1.00	18.65 A
1	.0	ATOM	2028	N	LYS A	Α	337	85.808	15.244	-15.688	1.00	18.38 A
		ATOM	2029	CA	LYS A	A	337	86.821	14.240	-15.387	1.00	18.89 A
		ATOM	2030	СВ	LYS A	Α	337	86.147	12.900	-15.082	1.00	17.70 A
		MOTA	2031	CG	LYS A	A	337	85.460	12.933	-13.727	1.00	19.89 A
		MOTA	2032	CD	LYS Z	A	337	84.450	11.817	-13.523	1.00	22.66 A
1	5	ATOM	2033	CE	LYS A	A	337	85.089	10.453	-13.372	1.00	22.78 A
		ATOM	2034	NZ	LYS A	A	337	84.025	9.444	-13.088	1.00	25.28 A
		ATOM	2035	С	LYS A	A	337	87.865	14.101	-16.504	1.00	20.07 A
		ATOM	2036	0	LYS A	A	337	88.996	13.671	-16.254	1.00	20.47 A
		ATOM	2037	N	ALA A	A		87.491	14.486	-17.725		20.38 A
2	20	ATOM	2038	CA	ALA A			88.393	14.441	-18.876	1.00	20.65 A
		ATOM	2039	СВ	ALA A			87.580		-20.178		20.29 A
		ATOM	2040	С	ALA A			89.357		-18.933		22.18 A
		ATOM	2041	0	ALA A			90.265		-19.768		24.71 A
		ATOM	2042	N	HIS A			89.179		-18.063		21.90 A
2		ATOM	2043	CA	HIS A			90.072		-18.094		22.10 A
		ATOM	2044	СВ	HIS A			89.711		-16.989		21.35 A
		ATOM	2045	CG	HIS A			90.357		-17.149		20.57 A
		ATOM	2046		HIS A			89.891		-17.683		19.19 A
,		ATOM	2047		HIS A			91.664		-16.783		20.52 A
3		ATOM ATOM	2048 2049		HIS A			91.973 90.914		-17.085 -17.633		22.28 A 21.96 A
		ATOM	2049	C	HIS A			91.555		-17.963		22.78 A
		ATOM	2051	0	HIS Z			91.919		-17.118		21.05 A
		ATOM	2052	N	PRO Z			92.425		-18.801		24.12 A
3		ATOM	2053	CD	PRO Z			92.090		-19.855		23.53 A
		ATOM	2054	CA	PRO Z			93.872		-18.795		25.11 A
		ATOM	2055	СВ	PRO Z			94.435		-19.647		22.31 A
		ATOM	2056	CG	PRO Z			93.379		-20.685		22.50 A
		ATOM	2057	С	PRO A			94.540		-17.421		25.66 A
4	10	ATOM	2058	0	PRO Z	A	340	95.523	16.951	-17.237	1.00	27.43 A
		ATOM	2059	N	PHE Z	A	341	94.011	18.389	-16.459	1.00	25.05 A
		ATOM	2060	CA	PHE Z	A	341	94.596	18.399	-15.139	1.00	24.88 A
		MOTA	2061	СВ	PHE Z	A		93.897	19.459	-14.276	1.00	24.71 A
		MOTA	2062	CG	PHE Z	A	341	94.482	19.607	-12.893		24.42 A
4	15	ATOM	2063	CD1	PHE Z	A	341	95.822		-12.721	1.00	22.55 A
		MOTA	2064	CD2	PHE Z	A	341	93.685		-11.758		22.61 A
		MOTA	2065		PHE Z			96.364		-11.434		23.65 A
		ATOM	2066		PHE Z			94.204		-10.476		22.09 A
_		ATOM	2067	CZ	PHE Z			95.547		-10.304		24.01 A
5		ATOM	2068	С	PHE Z			94.511		-14.486		25.70 A
		ATOM	2069	0	PHE Z			95.363		-13.680		27.11 A
		ATOM	2070	N	PHE Z			93.499		-14.865		25.51 A
		ATOM	2071	CA	PHE Z			93.262		-14.318		25.34 A
_	_	ATOM	2072	CB	PHE A			91.758		-14.120		21.93 A
5		ATOM	2073	CG	PHE A			91.120		-13.196		20.26 A
		ATOM	2074		PHE A			91.556		-11.888		20.03 A
		ATOM	2075		PHE A			90.030		-13.613		19.36 A
		ATOM	2076 2077		PHE A			90.907 89.377		-11.004 -12.744		19.87 A
		ATOM	2011	CEZ	PHE Z	Η.	J44	09.3//	11.340	-144	1.00	18.17 A

	MOTA	2078	CZ	PHE	Α	342	89.818	17.470	-11.431	1.00	19.27	Α
	ATOM	2079	С	PHE	Α	342	93.805	13.815	-15.214	1.00	27.64	Α
	ATOM	2080	0	PHE	Α	342	93.508	12.630	-15.019	1.00	27.39	Α
	ATOM	2081	N	GLU	Δ	343	94.607	14.203	-16.194	1.00	31.32	Δ
5	ATOM	2082	CA	GLU			95.185		-17.150		34.29	
5		2082		GLU								
	ATOM		CB				96.320		-17.889		38.36	
	ATOM	2084	CG	GLU			96.735		-19.197		45.23	
	MOTA	2085	CD	GLU	Α	343	97.654		-19.976		51.01	
	ATOM	2086	OE1	GLU	Α	343	98.266	13.801	-20.981	1.00	51.76	Α
10	ATOM	2087	OE2	GLU	Α	343	97.755	15.439	-19.568	1.00	52.42	Α
	ATOM	2088	С	GLU	Α	343	95.690	11.950	-16.542	1.00	33.50	Α
	ATOM	2089	0	GLU			95.289	10.860	-16.970		33.57	
	ATOM	2090	N	SER			96.554		-15.537		31.58	
	ATOM	2090	CA	SER			97.117		-14.906		30.38	
1.5												
15	ATOM	2092	СВ	SER			98.447		-14.253		29.76	
	ATOM	2093	OG	SER			98.243		-13.096		30.32	
	ATOM	2094	С	SER	Α	344	96.242	10.150	-13.857	1.00	30.00	Α
	ATOM	2095	0	SER	Α	344	96.662	9.137	-13.285	1.00	31.14	Α
	ATOM	2096	N	VAL	Α	345	95.046	10.679	-13.606	1.00	27.28	Α
20	ATOM	2097	CA	VAL	Α	345	94.135	10.126	-12.609	1.00	25.39	Α
	ATOM	2098	СВ	VAL			93.093		-12.159		24.17	
	ATOM	2099		VAL			91.973		-11.347		19.50	
	ATOM	2100		VAL			93.779		-11.363		17.85	
				VAL								
25	ATOM	2101	C				93.341		-13.043		26.45	
25	ATOM	2102	0	VAL			92.813		-14.154		27.42	
	ATOM	2103	N	THR			93.253		-12.157		26.62	
	MOTA	2104	CA	THR	Α	346	92.451		-12.406		27.91	
	ATOM	2105	CB	THR	Α	346	93.194	5.388	-11.999	1.00	29.18	Α
	ATOM	2106	OG1	THR	Α	346	94.345	5.224	-12.830	1.00	33.51	Α
30	ATOM	2107	CG2	THR	Α	346	92.300	4.171	-12.177	1.00	28.24	Α
	ATOM	2108	С	THR	Α	346	91.229	6.856	-11.505	1.00	27.53	Α
	ATOM	2109	0	THR			91.297		-10.299		29.24	
	ATOM	2110	N	TRP			90.117		-12.094		27.83	
		2111									29.15	
25	ATOM		CA	TRP			88.898		-11.336			
35	ATOM	2112	СВ	TRP			87.878		-12.224		27.12	
	ATOM	2113	CG	TRP			88.353		-12.758		25.48	
	MOTA	2114	CD2	TRP	Α	347	88.252		-12.118	1.00	24.27	Α
	MOTA	2115	CE2	TRP	Α	347	88.841	11.803	-12.990	1.00	23.82	Α
	MOTA	2116	CE3	TRP	Α	347	87.723	11.292	-10.897	1.00	22.42	Α
40	ATOM	2117	CD1	TRP	Α	347	88.984	9.788	-13.952	1.00	24.47	Α
	ATOM	2118	NE1	TRP	Α	347	89.279	11.124	-14.099	1.00	23.92	А
	ATOM	2119	CZ2				88.913	13.169	-12.678		21.68	
	ATOM			TRP			87.797		-10.586		24.15	
	ATOM	2121		TRP			88.391		-11.480		22.35	
45		2122	C						-10.700			
43	ATOM			TRP			88.218				30.64	
	ATOM	2123	0	TRP			87.617		-9.631		31.21	
	ATOM	2124	N	GLU			88.318		-11.376		32.16	
	ATOM	2125	CA	GLU	Α	348	87.698		-10.952		34.98	
	MOTA	2126	СВ	GLU	Α	348	88.157	2.890	-11.904	1.00	37.47	Α
50	ATOM	2127	CG	GLU	Α	348	87.815	3.125	-13.419	1.00	41.39	Α
	ATOM	2128	CD	GLU	Α	348	88.619	4.257	-14.116	1.00	41.83	Α
	ATOM	2129	OE1	GLU	Α	348	89.828	4.408	-13.841	1.00	42.27	Α
	ATOM	2130		GLU			88.036		-14.959		42.41	
	ATOM	2131	C	GLU			87.843		-9.478		34.74	
55		2132	0	GLU			86.866	3.111	-8.869		35.95	
55	MOTA											
	ATOM	2133	N	ASN			89.024	3.652	-8.887		33.61	
	ATOM	2134	CA	ASN			89.189	3.179	-7.507		32.34	
	ATOM	2135	СВ	ASN			89.936	1.860	-7.529		33.21	
	ATOM	2136	CG	ASN	A	349	91.345	2.016	-8.089	1.00	34.48	A

	7.50.7.6	0107	OD 1	7. (2.3.1	_	240	01 (12	0 043	0 0 5 0	1 00 20 01 7
	ATOM	2137		ASN			91.613	2.943	-8.858	1.00 32.91 A
	ATOM	2138		ASN			92.247	1.110	-7.712	1.00 35.85 A
	MOTA	2139	С	ASN			89.949	4.136	-6.594	1.00 31.22 A
	ATOM	2140	0	ASN	Α	349	90.826	3.714	-5.839	1.00 31.07 A
5	ATOM	2141	N	LEU	Α	350	89.611	5.416	-6.646	1.00 28.54 A
	ATOM	2142	CA	LEU	Α	350	90.300	6.403	-5.837	1.00 26.75 A
	ATOM	2143	СВ	LEU			89.632	7.762	-6.024	1.00 25.89 A
	ATOM	2144	CG	LEU			90.095	8.558	-7.239	1.00 24.21 A
	ATOM	2145		LEU			89.111	9.674	-7.547	1.00 23.55 A
10	ATOM	2146		LEU			91.475	9.118	-6.932	1.00 23.67 A
10										
	ATOM	2147	С	LEU			90.440	6.102	-4.345	1.00 27.67 A
	MOTA	2148	0	LEU			91.478	6.401	-3.753	1.00 28.06 A
	MOTA	2149	N	HIS			89.424	5.509	-3.722	1.00 27.81 A
	ATOM	2150	CA	HIS	Α	351	89.539	5.254	-2.299	1.00 29.88 A
15	ATOM	2151	СВ	HIS	Α	351	88.144	5.197	-1.646	1.00 31.47 A
	MOTA	2152	CG	HIS	Α	351	87.584	3.823	-1.475	1.00 32.65 A
	ATOM	2153	CD2	HIS	Α	351	86.926	3.009	-2.338	1.00 34.75 A
	MOTA	2154		HIS			87.629	3.150	-0.273	1.00 34.31 A
	ATOM	2155		HIS			87.022	1.981	-0.402	1.00 36.41 A
20	ATOM	2156		HIS			86.586	1.871	-1.644	1.00 35.36 A
20										
	ATOM	2157	C	HIS			90.396	4.030	-1.978	1.00 30.93 A
	ATOM	2158	0	HIS			90.674	3.741	-0.812	1.00 31.57 A
	MOTA	2159	N	GLN			90.842	3.337	-3.022	1.00 31.09 A
	ATOM	2160	CA	GLN			91.709	2.177	-2.864	1.00 31.86 A
25	MOTA	2161	СВ	GLN			91.482	1.187	-3.992	1.00 35.63 A
	ATOM	2162	CG	GLN	Α	352	91.038	-0.141	-3.497	1.00 40.62 A
	ATOM	2163	CD	GLN	Α	352	89.739	-0.036	-2.766	1.00 42.39 A
	ATOM	2164	OE1	GLN			88.684	0.133	-3.376	1.00 44.19 A
	ATOM	2165	NE2	GLN			89.802	-0.112	-1.447	1.00 44.81 A
30	ATOM	2166	C	GLN			93.167	2.626	-2.907	1.00 31.39 A
50	ATOM	2167	0	GLN			94.030	2.020	-2.271	1.00 31.33 A
		2168					93.429	3.685	-3.672	1.00 31.44 A
	ATOM		N	GLN						
	ATOM	2169	CA	GLN			94.769	4.237	-3.813	1.00 27.37 A
	ATOM	2170	СВ	GLN			94.767	5.283	-4.932	1.00 25.81 A
35	MOTA	2171	CG	GLN			94.250	4.702	-6.242	1.00 26.68 A
	ATOM	2172	CD	GLN	Α	353	94.035	5.738	-7.330	1.00 26.81 A
	ATOM	2173	OE1	GLN	Α	353	94.792	6.709	-7.435	1.00 25.21 A
	ATOM	2174	NE2	GLN	Α	353	93.011	5.520	-8.171	1.00 24.24 A
	MOTA	2175	С	GLN	Α	353	95.288	4.851	-2.510	1.00 28.25 A
40	ATOM	2176	0	GLN	Α	353	94.511	5.245	-1.633	1.00 28.38 A
	ATOM	2177	N	THR	Α	354	96.608	4.907	-2.375	1.00 28.16 A
	ATOM	2178	CA	THR			97.220	5.489	-1.193	1.00 28.54 A
	ATOM	2179	СВ	THR			98.564	4.848	-0.889	1.00 29.50 A
	ATOM	2180		THR			98.354	3.459	-0.624	1.00 31.62 A
45	ATOM	2181		THR			99.225	5.517	0.334	1.00 31.02 A
43										
	ATOM	2182	С	THR			97.438	6.955	-1.468	1.00 27.76 A
	MOTA	2183	0	THR			98.062	7.307	-2.453	1.00 27.12 A
	MOTA	2184	N	PRO			96.928	7.832	-0.592	1.00 28.37 A
	ATOM	2185	CD	PRO			96.067	7.582	0.573	1.00 27.67 A
50	ATOM	2186	CA	PRO	Α	355	97.092	9.266	-0.802	1.00 28.53 A
	ATOM	2187	СВ	PRO	Α	355	96.215	9.883	0.291	1.00 28.29 A
	ATOM	2188	CG	PRO	Α	355	95.210	8.807	0.579	1.00 28.38 A
	MOTA	2189	С	PRO			98.528	9.724	-0.695	1.00 28.85 A
	ATOM	2190	0	PRO			99.290	9.232	0.139	1.00 29.42 A
55	ATOM	2191	N	PRO			98.916	10.676	-1.548	1.00 29.42 A 1.00 28.20 A
55										
	ATOM	2192	CD	PRO			98.083	11.340	-2.567	1.00 27.35 A
	ATOM	2193	CA	PRO			100.276	11.213	-1.539	1.00 28.63 A
	ATOM	2194	СВ	PRO			100.261	12.199	-2.712	1.00 29.02 A
	ATOM	2195	CG	PRO	Α	356	98.815	12.633	-2.781	1.00 27.44 A

	ATOM	2196	С	PRO	Δ	356	100.483	11.899	-0.195	1.00	29.18	Δ
	ATOM	2197	0	PRO			99.543	12.505	0.331		28.80	
	ATOM	2198	N	ALA			101.689	11.806	0.368		29.69	
	ATOM	2199	CA	ALA			101.942	12.439	1.664		31.97	
5	ATOM	2200	СВ	ALA	Α	357	103.273	11.964	2.253	1.00	29.11	Α
	ATOM	2201	С	ALA	Α	357	101.928	13.964	1.528	1.00	33.61	Α
	ATOM	2202	0	ALA			102.371	14.507	0.520		33.81	
	ATOM	2203	N	LEU			101.390	14.645	2.540		36.37	
											38.03	
10	ATOM	2204	CA	LEU			101.295	16.110	2.543			
10	ATOM	2205	СВ	LEU			99.995	16.554	3.209		36.49	
	MOTA	2206	CG	LEU	Α	358	98.679	16.059	2.641		35.57	
	ATOM	2207	CD1	LEU	Α	358	97.568	16.398	3.620	1.00	35.78	Α
	MOTA	2208	CD2	LEU	Α	358	98.443	16.689	1.278	1.00	37.10	Α
	ATOM	2209	С	LEU	Α	358	102.460	16.743	3.310	1.00	39.05	Α
15	ATOM	2210	0	LEU			102.451	16.592	4.553		39.24	
13	ATOM	2211		LEU			103.348	17.370	2.679		40.12	
	ATOM	2212	OH2	TIP		1	82.347	32.462	-3.850		16.08	
	ATOM	2213	OH2		S	4	80.761		-18.244		23.37	
	ATOM	2214	OH2	TIP	S	7	79.269	13.051	-18.353	1.00	22.32	S
20	ATOM	2215	OH2	TIP	S	8	86.710	32.919	-1.646	1.00	24.05	S
	ATOM	2216	OH2	TIP	S	9	78.564	-0.823	16.465	1.00	28.00	S
	ATOM	2217		TIP	S	10	75.323	16.274	8.538		18.43	
	ATOM	2218	OH2	TIP	S	12	78.540	24.328	-2.128		27.08	
				TIP							22.56	
2.5	ATOM	2219	OH2		S	13	91.533		-17.231			
25	ATOM	2220	OH2	TIP	S	14	77.419	-0.445	24.044		23.98	
	ATOM	2221	OH2	TIP	S	19	72.498	40.164	-3.114		21.78	S
	MOTA	2222	OH2	TIP	S	20	77.303	13.198	-15.393	1.00	22.49	S
	ATOM	2223	OH2	TIP	S	21	75.600	-1.063	22.040	1.00	24.29	S
	ATOM	2224	OH2	TIP	S	22	90.133	19.697	12.606	1.00	16.61	S
30	ATOM	2225	OH2	TIP	S	24	74.810	7.002	5.700		20.66	
50	ATOM	2226	OH2	TIP	S	27	74.894	8.778	-8.074		23.31	
	ATOM	2227	OH2	TIP	S	28	80.070		-17.170		27.29	
	ATOM	2228	OH2	TIP	S	31	74.744	21.007	3.348		29.98	
	ATOM	2229	OH2	TIP	S	32	97.930	12.301	2.472	1.00	16.75	S
35	ATOM	2230	OH2	TIP	S	35	78.412	7.338	3.002	1.00	16.51	S
	ATOM	2231	OH2	TIP	S	36	80.172	27.171	1.300	1.00	34.66	S
	ATOM	2232	OH2	TIP	S	41	69.773	3.412	17.444	1.00	24.08	S
	ATOM	2233	OH2	TIP		43	88.878	7.904	10.616		20.34	
		2234	OH2	TIP	S	44	87.375		-13.928		31.99	
40	ATOM										35.59	
40	ATOM	2235	OH2	TIP	S	45	91.671		-16.123	1.00		
	ATOM	2236	OH2	TIP	S	46	87.637	11.564	23.703		22.67	
	MOTA	2237	OH2	TIP	S	48	93.353	28.739	3.547		32.79	
	ATOM	2238	OH2	TIP	S	50	82.283	34.597	-16.032	1.00	23.90	S
	MOTA	2239	OH2	TIP	S	52	81.673	8.965	-8.348	1.00	27.83	S
45	ATOM	2240	OH2	TIP	S	55	94.012	3.488	1.399		24.78	S
	ATOM	2241		TIP		58	85.735		-18.436		27.15	
	ATOM	2242		TIP		61	79.069	-4.638	12.345		21.04	
	ATOM	2243		TIP		64	103.981	17.563			28.86	
	ATOM	2244		TIP		66	79.020	43.119	5.431 3.079		33.30	
50	ATOM	2245	OH2	TIP	S	69	88.177	36.956	3.079	1.00	30.87	S
	ATOM	2246	OH2	TIP	S	75	78.707	27.486	-3.439	1.00	25.25	S
	ATOM	2247	OH2	TIP	S	79	80.347	33.345	6.422	1.00	38.57	S
	ATOM	2248		TIP		84	64.594	19.493	24.406		26.01	
	ATOM	2249		TIP		98	70.215	21.980	19.413		24.75	
55												
55	ATOM	2250		TIP			103.456	14.637	-2.925		41.84	
	ATOM	2251		TIP			97.528		-14.706		43.27	
	ATOM	2252		TIP			103.602		-1.388		37.07	
	ATOM	2253	OH2	TIP	S	129	83.353	33.273	4.410	1.00	34.78	S
	ATOM	2254	OH2	TIP	S	130	74.116	4.597	-3.022	1.00	27.69	S

	ATOM	2255	OH2	TIP	S	131	73.104	-1.689	21.760	1.00	32.76	S
	ATOM	2256	OH2	TIP		133	101.510	19.036	-1.083	1.00	28.30	S
	ATOM	2257	он2	TIP		134	65.138	6.209	20.472	1.00	27.43	S
	ATOM	2258	OH2	TIP	S	135	94.509		-12.734		40.27	
5	ATOM	2259	OH2	TIP	S	136	76.896		-17.698			S
5									-6.673			
	ATOM	2260	OH2	TIP	S	137	97.379	7.497				
	ATOM	2261	OH2	TIP		138	62.239	17.934	24.368		34.35	
	ATOM	2262	OH2		S	139	69.630		-10.771		38.17	
	MOTA	2263	OH2	TIP	S	140	84.554	44.493	-2.658		24.74	
10	MOTA	2264	OH2	TIP	S	141	94.631	8.129	-9.752	1.00	35.45	S
	ATOM	2265	OH2	TIP	S	142	78.415	1.021	3.883	1.00	28.60	S
	ATOM	2266	OH2	TIP	S	143	99.830	12.987	-10.148	1.00	35.79	S
	ATOM	2267	OH2	TIP	S	144	71.235	20.688	11.365		51.52	
	ATOM	2268	OH2	TIP	S	145	87.138	25.623	11.165		41.92	
15	ATOM	2269	OH2	TIP	S	146	60.803	15.332	23.294		32.69	
13		2270	OH2	TIP		148	73.970		-13.455		33.99	
	ATOM											
	ATOM	2271	OH2		S	149	88.146	19.004	17.326		27.60	
	ATOM	2272	OH2	TIP		150	90.803	9.970	18.127		35.03	
	ATOM	2273	OH2	TIP	S	153	86.261		-16.403	1.00	41.89	S
20	MOTA	2274	OH2	TIP	S	155	102.147	7.767	-0.215	1.00	38.83	S
	ATOM	2275	OH2	TIP	S	159	95.238	0.811	-7.614	1.00	47.22	S
	ATOM	2276	OH2	TIP	S	163	92.356	36.543	-5.580	1.00	40.19	S
	ATOM	2277	OH2	TIP	S	172	66.640	4.633	22.314	1.00	29.95	S
	ATOM	2278	OH2	TIP	S	176	99.303	9.124	3.136		37.07	
25	ATOM	2279	OH2	TIP		184	104.566	20.517	-7.318		40.83	
23		2280	OH2	TIP	S	185	90.295		-15.433		34.81	
	ATOM											
	ATOM	2281	OH2		S	186	82.626	12.831	8.023		23.99	
	ATOM	2282	OH2	TIP	S	187	86.159	18.737	24.618		32.12	
	ATOM	2283	OH2	TIP		188	79.867	7.010	-7.877		28.52	
30	ATOM	2284	OH2	TIP	S	189	88.469	4.967	1.404		45.39	S
	MOTA	2285	OH2	TIP	S	190	95.628	28.435	-17.705	1.00	31.73	S
	ATOM	2286	OH2	TIP	S	191	76.228	7.822	28.547	1.00	36.76	S
	ATOM	2287	OH2	TIP	S	192	85.930	8.936	23.323	1.00	31.58	S
	ATOM	2288	OH2	TIP	S	193	73.669	24.555	-14.317	1.00	34.12	S
35	ATOM	2289	OH2	TIP	S	194	99.847	12.959	4.319		43.06	
	ATOM	2290	OH2	TIP	S	195	76.225	28.669	-3.386			S
	ATOM	2291	OH2	TIP	S	197	76.955	24.214	20.057		35.16	
	ATOM	2292	OH2	TIP		198	65.723	11.313	28.926		38.40	
40	ATOM	2293	OH2	TIP	S	199	88.482	28.463	4.472		29.21	
40	ATOM	2294	OH2		S	200	71.017		-13.980	1.00		S
	ATOM	2295	OH2	TIP		201	64.967	12.265	13.947			
	MOTA	2296		TIP			99.611				46.97	
	ATOM	2297	OH2	TIP	S	205	65.422	-1.944			65.13	
	MOTA	2298	OH2	TIP	S	210	89.648	5.683		1.00	38.65	S
45	ATOM	2299	OH2	TIP	S	213	80.842	40.555	7.721	1.00	37.38	S
	ATOM	2300	OH2	TIP	S	214	77.452	22.142	23.411	1.00	36.35	S
	ATOM	2301		TIP			104.280		-10.347		35.15	
	ATOM	2302		TIP			84.900	44.787			36.10	
	ATOM	2303		TIP			74.759	19.808	9.165		29.67	
50												
30	ATOM	2304		TIP			76.375	2.991	-2.919		33.34	
	ATOM	2305		TIP			97.252		-15.430		39.17	
	ATOM	2306		TIP			70.180	4.692	8.907		29.97	
	MOTA	2307		TIP			96.055	11.349	-8.926	1.00	29.40	S
	ATOM	2308	OH2	TIP	S	235	70.916	31.535	4.186	1.00	53.99	S
55	ATOM	2309	OH2	TIP	S	236	83.279	23.905	15.245	1.00	40.79	S
	ATOM	2310		TIP			90.441	34.500	3.752		37.91	
	ATOM	2311		TIP			74.369		-11.954		36.85	
	ATOM	2312		TIP				5.971			48.63	
	ATOM	2313		TIP			101.866	29.649	1.029		48.93	
	111011	2010	V11Z	E	D	210	101.000	20.010	1.029	1.00	10.23	U

	ATOM	2314	012	GLC	G	2	74.980	15.310	28.834	1.00	58.25	G
	ATOM	2315	C11	GLC	G	2	74.113	15.072	27.724	1.00	58.49	G
	ATOM	2316	C13	GLC	G	2	74.885	14.362	26.609	1.00	58.11	G
						2			25.524			
_	ATOM	2317			G		73.990	14.120			58.57	
5	ATOM	2318	C15	GLC	G	2	75.438	13.023	27.096	1.00	57.55	G
	ATOM	2319	016	GLC	G	2	74.357	12.183	27.507	1.00	57.24	G
	ATOM	2320	012	GLC	G	3	68.191	4.312	13.268	1.00	63.76	G
		2321		GLC		3		3.273			63.57	
	ATOM						67.998		14.231			
	ATOM	2322	C13	GLC	G	3	69.274	2.429	14.330	1.00	64.06	G
10	ATOM	2323	014	GLC	G	3	69.570	1.858	13.049	1.00	62.75	G
	ATOM	2324	C1.5	GLC	G	3	69.094	1.303	15.364	1.00	63.85	G
						3						
	MOTA	2325		GLC			68.010	0.444	14.978		65.65	
	MOTA	2326	012	GLC	G	4	87.921	37.473	-13.378	1.00	46.73	G
	ATOM	2327	C11	GLC	G	4	88.767	36.757	-14.265	1.00	46.84	G
15	ATOM	2328	C13	GLC	G	4	90.050	36.439	-13.526	1.00	46.74	G
	ATOM	2329		GLC		4	90.660		-13.104		46.91	
	ATOM	2330	C15	GLC	G	4	90.999	35.678	-14.435	1.00	47.60	G
	ATOM	2331	016	GLC	G	4	92.193	35.413	-13.700	1.00	50.48	G
	ATOM	2332	012	GLC	G	6	78.608	8.519	28.683	1.00	42.02	G
20	ATOM	2333		GLC		6	79.227	8.721	29.956		44.70	
20												
	ATOM	2334		GLC		6	80.218	9.877	29.849		45.13	
	ATOM	2335	014	GLC	G	6	81.208	9.537	28.896	1.00	47.43	G
	ATOM	2336	C15	GLC	G	6	80.904	10.129	31.180	1.00	46.92	G
	ATOM	2337		GLC		6	81.611	8.950	31.564		49.38	
25												
25	MOTA	2338		GLC		8	83.278	5.163	12.485		46.74	
	ATOM	2339	C11	GLC	G	8	82.460	3.987	12.559	1.00	50.09	G
	ATOM	2340	C13	GLC	G	8	83.236	2.894	13.286	1.00	50.09	G
	ATOM	2341	014	GLC	G	8	84.408	2.621	12.529	1.00	50.75	G
	ATOM	2342		GLC		8	82.412	1.597	13.414		52.04	
20												
30	MOTA	2343		GLC		8	82.051	1.062	12.130		53.37	
	ATOM	2344	012	GLC	G	10	87.146	4.682	-5.006	1.00	25.46	G
	ATOM	2345	C11	GLC	G	10	85.823	5.086	-5.356	1.00	27.64	G
	ATOM	2346	C13	GLC	G	10	85.782	5.498	-6.835	1.00	30.79	G
	ATOM	2347			G	10	86.689	6.600	-7.069		29.47	
2.5												
35	MOTA	2348		GLC		10	84.354	5.916	-7.219		30.60	
	MOTA	2349	016	GLC	G	10	83.947	7.022	-6.417	1.00	31.23	G
	ATOM	2350	CBI	DRG	L	1	82.223	19.878	9.473	1.00	17.56	L
	ATOM	2351		DRG		1	82.835	19.573	10.730		20.33	
		2351										
	MOTA			DRG		1	82.419	20.512	11.733		17.87	
40	ATOM	2353	CBF	DRG	L	1	83.661	21.291	12.177	1.00	16.47	L
	ATOM	2354	NBK	DRG	L	1	84.171	22.133	11.085	1.00	15.68	L
	ATOM	2355	СВЈ	DRG	T.	1	83.683	23.479	10.751	1.00	12.47	T.
	ATOM	2356		DRG		1	84.739	20.294	12.600		16.76	
	ATOM	2357		DRG		1	84.178	19.405	13.715		18.27	
45	ATOM	2358	OBB	DRG	$_{ m L}$	1	82.790	19.632	14.017	1.00	18.03	L
	ATOM	2359	CBC	DRG	L	1	81.853	19.747	12.937	1.00	18.62	L
	ATOM	2360		DRG		1	80.732	20.611	13.524		14.59	
	MOTA	2361		DRG		1	81.398	18.547	12.551		18.60	
	ATOM	2362	CAX	DRG	L	1	80.185	18.344	12.014	1.00	15.55	L
50	ATOM	2363	CAY	DRG	L	1	79.107	19.141	11.643	1.00	13.82	L
	ATOM	2364		DRG		1	77.988	18.555	11.053		16.37	
						1			10.830		15.88	
	ATOM	2365		DRG			77.930	17.180				
	MOTA	2366		DRG		1	78.999	16.366	11.196		15.07	
	MOTA	2367	CAN	DRG	L	1	80.107	16.973	11.783	1.00	17.80	L
55	ATOM	2368		DRG		1	81.290	16.377	12.187	1.00	19.34	L
						1						
	ATOM	2369		DRG			81.811	15.087	12.083		19.93	
	ATOM	2370		DRG		1	82.083	17.407	12.657		18.53	
	ATOM	2371	CAU	DRG	L	1	83.404	17.144	13.014	1.00	18.70	L
	ATOM	2372	NAT	DRG	L	1	84.365	17.964	13.438	1.00	17.82	L

	MOTA	2373	CAS	DRG	L	1	85.523	17.317	13.610	1.00 15.80 L
	ATOM	2374	CAR	DRG	L	1	86.807	17.682	14.000	1.00 14.23 L
	ATOM	2375	CAQ	DRG	L	1	87.803	16.708	14.047	1.00 13.92 L
	ATOM	2376	CAI	DRG	L	1	87.526	15.384	13.714	1.00 16.21 L
5	ATOM	2377	CAJ	DRG	L	1	86.244	15.003	13.324	1.00 16.43 L
	ATOM	2378	CAK	DRG	L	1	85.264	15.988	13.278	1.00 17.76 L
	ATOM	2379	CAL	DRG	L	1	83.932	15.867	12.904	1.00 18.99 L
	ATOM	2380	CAG	DRG	L	1	83.130	14.829	12.439	1.00 19.47 L
	ATOM	2381	CAC	DRG	L	1	83.403	13.472	12.290	1.00 18.70 L
10	ATOM	2382	OAB	DRG	L	1	84.471	12.895	12.480	1.00 18.10 L
	ATOM	2383	NAD	DRG	L	1	82.277	12.904	11.856	1.00 18.49 L
	ATOM	2384	CAE	DRG	L	1	81.128	13.799	11.622	1.00 20.08 L
	ATOM	2385	OAF	DRG	L	1	80.902	13.891	10.214	1.00 24.92 L
	ATOM	2386	S	SO4	Ι	1	64.638	8.174	16.414	1.00 89.13 I
15	ATOM	2387	01	SO4	I	1	65.311	9.465	16.666	1.00 88.78 I
	ATOM	2388	02	SO4	I	1	63.197	8.413	16.200	1.00 89.62 I
	ATOM	2389	03	SO4	I	1	64.827	7.262	17.566	1.00 88.49 I
	ATOM	2390	04	SO4	I	1	65.197	7.555	15.196	1.00 89.77 I
	ATOM	2391	S	SO4	I	3	84.884	-1.751	12.531	1.00 81.17 I
20	ATOM	2392	01	SO4	I	3	84.762	-0.302	12.775	1.00 81.32 I
	ATOM	2393	02	SO4	I	3	84.538	-2.490	13.758	1.00 81.49 I
	ATOM	2394	03	SO4	I	3	86.280	-2.053	12.162	1.00 81.73 I
	ATOM	2395	04	SO4	I	3	83.976	-2.163	11.440	1.00 81.19 I
	ATOM	2396	S	SO4	I	5	74.420	22.898	12.677	1.00 85.50 I
25	ATOM	2397	01	SO4	Ι	5	73.256	22.153	12.161	1.00 85.36 I
	ATOM	2398	02	SO4	I	5	75.637	22.104	12.412	1.00 84.51 I
	ATOM	2399	03	SO4	Ι	5	74.250	23.138	14.126	1.00 84.13 I
	ATOM	2400	04	SO4	I	5	74.527	24.202	11.997	1.00 85.44 I
	ATOM	2401	S	SO4	Ι	6	68.798	6.993	-3.457	1.00 73.84 I
30	ATOM	2402	01	SO4	I	6	68.338	7.338	-4.823	1.00 72.86 I
	ATOM	2403	02	SO4	I	6	69.298	8.206	-2.791	1.00 73.61 I
	ATOM	2404	03	SO4	I	6	69.888	6.003	-3.540	1.00 73.52 I
	ATOM	2405	04	SO4	I	6	67.690	6.426	-2.658	1.00 73.19 I
	ATOM	2406	02	PO4	Ρ	100	66.501	25.721	2.616	1.00 85.98 P
35	ATOM	2407	03	PO4	Ρ	100	64.376	25.028	1.654	1.00 86.96 P
	ATOM	2408	04	PO4		100	65.755	26.653	0.496	1.00 86.51 P
	ATOM	2409	01	PO4	Ρ	100	64.621	27.279	2.570	1.00 86.98 P
	ATOM	2410	P	PO4		100	65.315	26.170	1.832	1.00 87.36 P
	ATOM	2411	S	so4		3	80.775	-0.045	7.874	0.50 22.29 X
40	ATOM	2412	01	SO4		3	81.160	0.521	9.176	0.50 22.30 X
•	ATOM	2413	02	SO4		3	81.320	-1.407	7.778	0.50 22.49 X
	ATOM	2414	03	SO4		3	81.309	0.781	6.777	0.50 23.26 X
	ATOM	2415	04	SO4		3	79.305	-0.088	7.772	0.50 24.36 X
	END					-				
45										